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**Documentation and Analysis of a
Global CO₂ Model**

Developed by Peng et al. (1983)

H.I. Jager
T.H. Peng
A. W. King
M.J. Sale

ENVIRONMENTAL SCIENCES DIVISION
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ABSTRACT

A global carbon model, the Peng '83 model, has been standardized according to protocols developed for an intermodel comparison. The first part of this document describes the model as we received it, and the second part describes a standardized version of the model, which has been parameterized according to the protocols described. Model performance was evaluated according to defined criteria and a sensitivity analysis of the model was conducted to identify the most important parameters.

The standardized model was supplemented with a calibration routine to define reasonable combinations of initial conditions. This improved the ability of the model to hold an initial equilibrium state. Sensitivity analysis showed a shift in parameter importances with time. The initial conditions were of greatest importance for the length of these simulations, but declined in longer simulations. With the initial $p\text{CO}_2$ excluded from the sensitivity analysis, ocean surface area (used to extrapolate results) was second in importance. While the CO_2 exchange rate were initially most important, the model projections of atmospheric CO_2 soon became more sensitive to the alkalinity of the ocean.

PART 1

THE ORIGINAL PENG '83 MODEL

1. DESCRIPTION

The Peng '83 model is a modification of the Oeschger et al. (1975) ocean model and is described in Peng et al. (1983). Like the Oeschger model, "it is a one-dimensional representation of the ocean. It includes CO₂ exchange between a well-mixed atmosphere and a well-mixed surface ocean reservoir and diffusive mixing into the waters lying below the mixed layer. . . . The CO₂ exchange rate and coefficient of vertical eddy diffusion are based on the distribution of natural radiocarbon in the system" (Peng et al. 1983). The Peng '83 model differs from the Oeschger model by modelling the production of deep water cycling from intermediate depths to the surface polar outcrop, down to the bottom and back up. In addition, oceanic primary productivity is incorporated in the Peng '83 model. Important modifications to parameter values were made by Peng et al. (1983) to match the observed penetration of bomb-produced tritium measured by the GEOSECS program. The conceptual framework of the model is shown in Fig. 1 (from Fig. 4 in Peng et al. 1983).

1.1 BACKGROUND

The source code for the Peng '83 model was obtained from Dr. Tsung Hung Peng in the Environmental Sciences Division at Oak Ridge National Laboratory in the fall of 1988. This code included three files, the main program (FFCO2), the subroutine REV, and the subroutine DPCO2X. Two input files were required, one with depth profiles for carbon and phosphorus, and one with the parameter values. Values for this second file were obtained from Peng et al. (1983). The original emissions inputs were replaced with the standardized emissions scenarios selected for this project. Previously, the final historical emissions level was projected into the future by specifying a fixed rate of future increase.

1.2 MODEL

The original Peng '83 model ocean represents an average one-dimensional ocean with 76 depth layers, each of which is 50 m thick. The model simulates changes in both carbon and phosphate in each depth layer over time. This difference equation model has concentrations of both carbon and phosphate for each of 76 depth layers, for a total of 152 state variables. Since most of the equations are the same for carbon and phosphates, descriptions are given only for carbon, unless the two are different.

The following processes are simulated at each time step in the simulation as shown in Fig. 2: (1) emissions are added to the atmosphere; (2) CO₂ is exchanged between the atmosphere and the two well-mixed surface layers, (3) diffusion takes place between successive depth layers in the ocean, (4) photosynthetic fixation of CO₂ is added as a decreasing function of depth, and (5) the advective polar outcrop cycle operates. The original Peng '83 follows the structure shown in Fig. 2, except for the call to

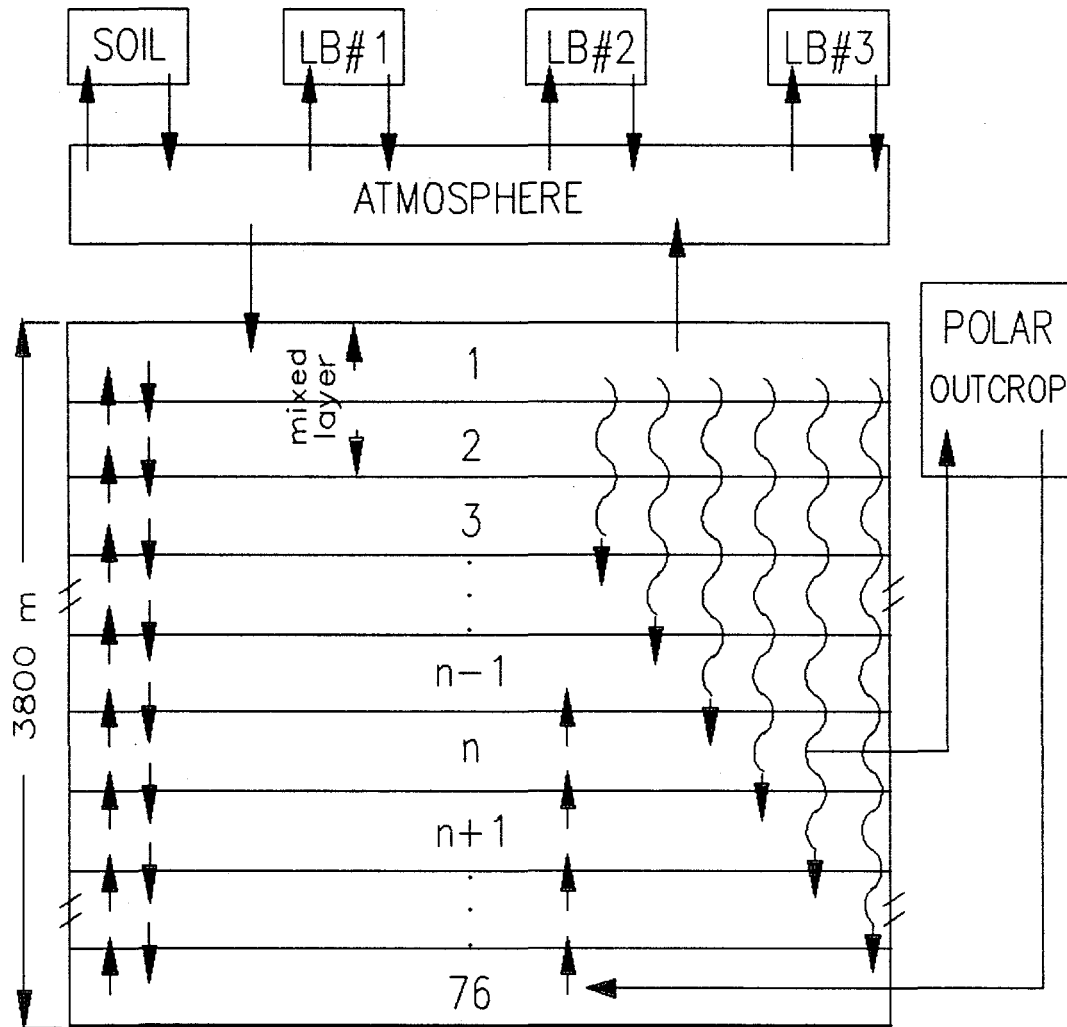


Figure 1. Multibox model used to calculate CO₂ uptake and carbon isotope dilution.

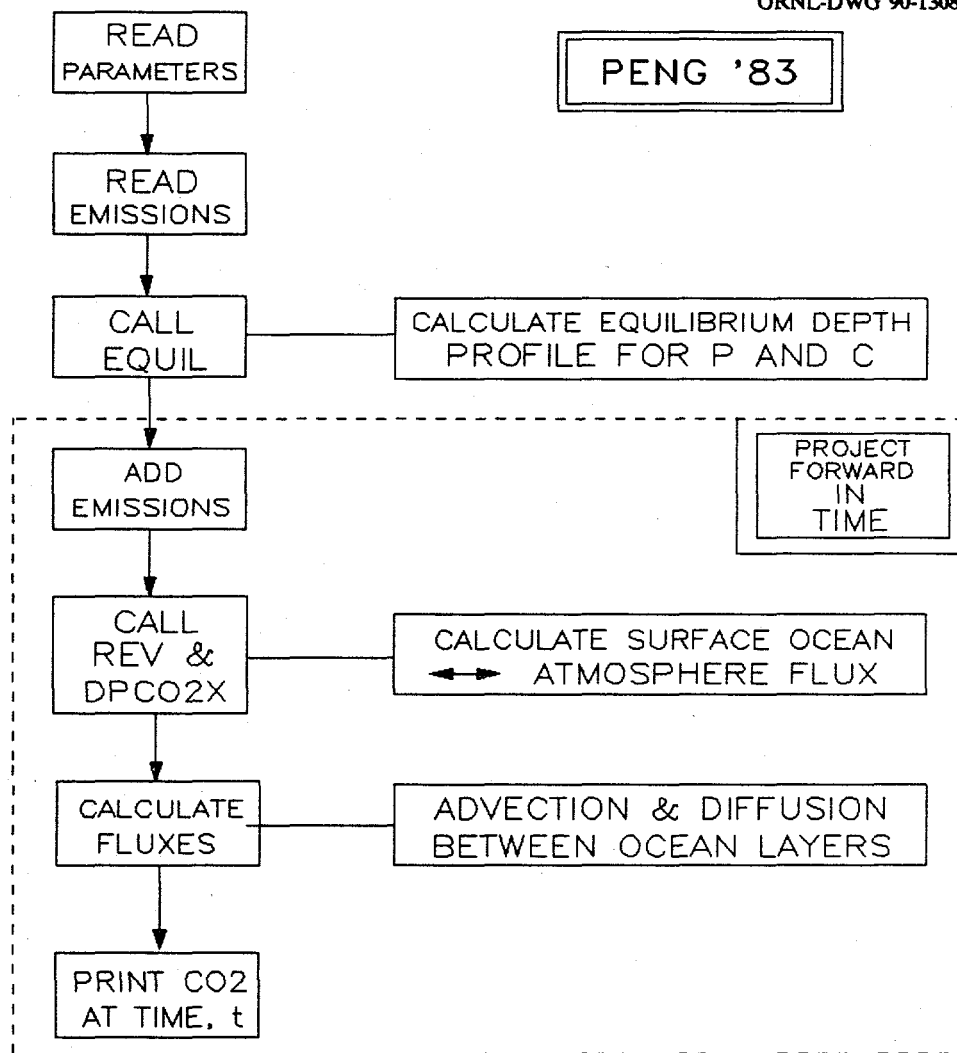


Figure 2. Flow chart illustrating the organization of the standardized Peng '83 model.

subroutine EQUIL (see Sect. 2.2). The biosphere fluxes across the top of Fig. 1 are not explicitly modelled, except through the emissions inputs. The exchange between the atmosphere and surface ocean is accomplished by using Takahashi's formulation for calculating the buffer or Revelle factor (Broecker et al., 1982). Changes in the partial pressure of CO₂ (pCO₂) of the surface ocean depend on average ocean salinity, temperature, alkalinity, and carbon. Diffusion of CO₂ is calculated as a linear flux between adjacent ocean layers.

The following equations summarize the difference equation model with the exception of the transfers between the atmosphere and surface ocean which go into the calculation of the Revelle factor, δ at each time step:

$$\begin{aligned} \Delta c_1 &= \Delta c_2 \\ &= \underset{\text{emissions}}{ff} + \underset{\text{diffusion}}{rk_2(c_3 - c_2)} - \underset{\text{photosynthesis}}{rk_2 p_3} \end{aligned} \quad [1]$$

$$\begin{aligned} \Delta c_k &= \underset{\text{diffusion}}{rk_{k-1}(c_{k-1} - c_k)} + \underset{\text{diffusion}}{rk_k(c_{k+1} - c_k)} + \underset{\text{advection}}{rw(c_{k+1} - c_k)} \\ &\quad + \underset{\text{photosynthesis}}{fb \cdot fp_k} \end{aligned} \quad [2]$$

$$\Delta c_{76} = \underset{\text{diffusion}}{rk_{75}(c_{k-1} - c_k)} + \underset{\text{advection}}{rw(c_{kd} - c_k - c_{CO2})} + \underset{\text{photosynthesis}}{fb \cdot fp_{76}} \quad [3]$$

$$\Delta pCO_{2a} = \underset{\text{emissions}}{ff} - \underset{\text{amount removed by ocean}}{(\sum c_k, k=1,76)(\text{volume of ocean})} \quad [4]$$

$$\Delta pCO_{2s} = \delta pCO_{2s} (\Delta c_1 / c_1) \quad [5]$$

The first two terms in Eq [2] represent the diffusion between depth layer k and the adjacent depth layers, above ($k - 1$) and below ($k + 1$). Removal of carbon by photosynthesis is modelled as a function of phosphate, whose concentration decays exponentially with depth (final term in Eq. [2]). The mixed layer is usually depleted of phosphate by photosynthetic activity and does not experience this loss in the current formulation.

There are two parts to the advective cycle, which involves only the deep ocean layers ($rw=0$ for depth layers above 700 m). Direct cold water injection into the deepest (76th) layer of ocean (the polar outcrop) is switched off in the version we obtained but can be switched on easily. The model version that we obtained has a more subtle advective process which simulates cold water advective fluxes along isohaline trajectories in the ocean; these fluxes inject CO₂ into the middle and deep layers and cause subsequent upwelling of that water. The advection cycle is accomplished by the third term in Eq.

[2] for layers below 700 m. This term adds carbon to any layer with a lower concentration than the layer below it, and removes carbon from those with relatively higher concentrations. The result is that carbon is added to layers just below 700 m and eroded from deeper layers until a peak is formed in the profile. Overall mass balance is maintained among deep ocean layers by removing $rw \cdot cco2$ from the 700 m ocean layer in the standardized version. This representation of deep water injection and upwelling is crucial to reproducing the peaked shape of GEOSECS depth profiles observed in most oceans.

1.3 IMPLEMENTATION OF THE MODEL

This model is a difference equation model written in ANSI standard FORTRAN. The original model uses time intervals of one-tenth of a year. A net carbon flux, $\Delta c_k(t)$, is determined for each depth layer, ($k = 3, 76$) on the basis of the processes listed above at each time step and added to the current concentration of carbon in the k th depth layer of the ocean. The basic difference equation for the intermediate depth layers is given by Eq. 2. The surface (Eq. 1) and bottom (Eq. 3) layer fluxes have somewhat different formulations. In addition, there is no advection term for the layers above the thermocline. The surface or mixed layers have different equations, because they incorporate the results of the surface-atmosphere exchanges. The last two equations, (Eq. 4 and 5), adjust the surface and atmosphere partial pressures at each time step. The time-variable Revelle factor controls the ocean surface uptake of emissions.

1.4 INITIAL PARAMETERIZATION

The original model is designed to start in the year 1860 with 280 ppm of atmospheric CO_2 . The initial parameter values appear in Peng et al. (1983) and are listed in Table 1. Dr. Peng provided the initial carbon and phosphorus profiles used in a file matching the original input format of the model (see Appendix A).

Table 1. Parameter values of the original Peng '83 model

Parameter	Description	Nominal value
AREA	Total ocean surface area	$360.0 \cdot 10^{12} \text{ m}^2$
CCO2	Polar CO ₂ reaching bottom water	$0.0 \text{ mol} \cdot \text{m}^{-3}$
DD	Depth of deep water origin	1000.0 m
DKL	Depth of thermocline	700.0 m
EI	Sea surface CO ₂ exchange rate	$17.0 \text{ mol} \cdot \text{m}^{-2} \cdot \text{year}^{-1}$
EK	Ocean thermocline diffusivity coefficient	$1.6 \text{ cm}^2 \cdot \text{s}^{-1}$
EKL	Deep sea diffusivity coefficient	$0.5 \text{ cm}^2 \cdot \text{s}^{-1}$
FD	Deep water flux by advection	50.0 sv
PCO2	Initial atmospheric CO ₂	280.0 ppm
PPMPM	Conversion from teramoles	$280.0 \cdot 50,000^{-1}$
S	Global average ocean salinity	35.0 ppt
TW	Global average sea surface temperature	20.0°C
TALK	Titration ocean alkalinity	$0.00233 \text{ equiv.} \cdot \text{kg}^{-1}$
TCO2	Titration total CO ₂ ($\text{mol} \cdot \text{kg}^{-1}$)	0.001969698

2. MODEL VERIFICATION: METHODS

2.1 BASIS FOR VERIFICATION

The goal of the verification procedure is to provide a bridge between (1) past scientific results based on the original model and (2) intermodel standardization needed to document and compare the original model with other reputable global CO₂ models. The replicability of scientific results is compromised if this link is ignored. Modeling is an iterative, evolving process; thus, successive papers using a single model in the scientific literature rarely refer to the same static model. One objective of the present implementation procedure is to document the differences between the original and the standardized versions of the model to ensure that the behavior of the standardized version is the intent of the model's authors. A second objective is to identify key processes that change the dynamic behavior of the model through a sensitivity analysis of the standardized model.

Sections 2.2-2.5 describe methods for documenting the behavior of the original Peng '83 model. Methods have been developed for summarizing model projections through the use of statistics that are meaningful to the scientific community and that are generally reported in the literature. We can use these statistics to compare our implementation of the original model with previously reported attributes of the model to ensure that we have a reasonable implementation of the original model. We will also use these statistics as a basis for documenting differences between the original model and the standardized version.

2.2 EQUILIBRATION TEST

The first test applied to the original Peng '83 model is a check on whether it holds equilibrium with all compartments remaining at steady state concentrations. This is an indication that the model is balancing mass correctly and parameterized in a way that is consistent with the assumption of a preindustrial equilibrium atmosphere. The model is run from the year 1860 with no emissions input and the original model parameter values and predicted atmospheric CO₂ are checked to see if they remain at the initial pCO₂. In theory, when there are no fossil fuel emissions or other sources of atmospheric CO₂ over time, the concentrations of carbon in the ocean layers and atmosphere should remain constant. This important modeling assumption allows simulations to begin at a certain point in time without regard to the previous emissions history. It assumes that preindustrial emissions were low and relatively constant over a long period of time prior to the initial simulation date. Current debate suggests that emissions were already increasing before the year 1860 and thus promote an earlier starting date for simulations. One difference that we will implement in the standardized model will be to use an earlier starting date.

2.3 REPLICATION OF THE HISTORICAL CO₂ RECORD

Historical measurements of atmospheric CO₂ concentrations are available from the Mauna Loa Observatory in Hawaii for the period 1959-85 (Keeling 1983) and from an ice core taken at Siple Station, Antarctica ca. 1750-1972 (Neftel et al. 1985). Annual measurements are available in the Mauna Loa record, whereas the Siple record covers a much longer period with more sporadic measurements.

The original model simulated atmospheric CO₂ over the historical period 1860-1980, using the parameter values listed in Table 1. In one simulation, combined CO₂ emissions from both reconstructed fossil fuel and land use sources were used to drive the model. In a second simulation, the reconstructed land use emissions were removed, because these numbers were incompatible with the observed CO₂ record (Enting and Mansbridge 1987).

The simulations from these two cases (with and without land use emissions) were compared with the two available historical records of atmospheric CO₂. Several indices were defined in order to summarize the deviation of each simulated CO₂ trajectory from the two historical records. The maximum deviation bounds the distance between the trajectories, and the year in which the curves are farthest apart can indicate the shape of the curve. In addition, two measures of the average deviation were defined: the average absolute deviation and the square root of the sum of squared deviations (RMS, or root mean square deviation) between the trajectories. These measures are all in units of parts per million (ppm).

2.4 REPLICATION OF THE HISTORICAL AIRBORNE FRACTION

The airborne fraction is a popular and somewhat controversial index of model performance (Gardner and Trabalka 1985). This index measures the fraction of CO₂ emissions that remains in the atmosphere after a fixed time interval. Over the historical period, the airborne fraction calculated from model projections can be compared with the measured airborne fraction. This measured airborne fraction depends on historical CO₂ records (Mauna Loa and Siple), which are fairly well known, and also on the reconstructed historical emissions records for fossil fuel and land use. The confidence in these reconstructions, particularly that for land use, is not high. In this case, however, the same emissions denominator is used in calculating both the simulated and the measured airborne fraction, so the differences between the calculated values should reflect only the differences in projected CO₂.

Airborne fractions have various computational definitions. We have adopted the most common definition: the change in atmospheric CO₂ over a specified period of time, divided by the total amount of CO₂ emitted during that same time period. As we wish to compare model projections of the airborne fraction with the measured airborne fractions estimated from the Mauna Loa and Siple records, we calculate airborne fractions for the Mauna Loa period (1959-80) and the Siple period (1750-1980). The denominator includes all emissions input to the models. In the historical simulation

without land use, land use emissions are not included in either the simulation or the calculated airborne fraction.

2.5 CO₂ FORECASTS

Forecasts of future atmospheric CO₂ were made by using the original Peng '83 model. The original model was designed to use Keeling's (1973) fossil fuel emissions inputs over the historical period, followed by a constant percentage increase in future projections. To aid in comparison with the standardized model, we use Keeling's estimates of historical fossil fuel emissions (with new estimates from 1973 to the present) and combine them with reconstructed land use emission estimates from Houghton et al. (1983). The forecasts are projected into the future using nine future emissions scenarios described in Sect. 4.2.

Descriptive statistics characterizing each of the nine forecasts were defined. The maximum atmospheric CO₂ concentration over the entire simulation period and the year at which this maximum occurred are given for each scenario projection. For the future CO₂ projections of each emissions scenario, we also report the total airborne fraction over the simulated period as defined in Sect. 2.4.

The time to doubling is another index summarizing the atmospheric CO₂ projections of a model. Doubling times report the year during which the CO₂ concentration of the atmosphere reaches twice that of the reference year. Time to doubling is often calculated from the years when concentrations of atmospheric CO₂ were 300 and 340 ppm, respectively. In reporting doubling times, we use these concentrations as reference points. In addition, because the suite of CO₂ models currently used do not begin to diverge from one another until after the doubling time is reached, we report quadrupling times as well. The four indices reported here will be the years in which each CO₂ projection reaches reference concentrations of 600, 680, 1200, and 1360 ppm.

3. MODEL VERIFICATION: RESULTS AND DISCUSSION

3.1 EQUILIBRATION TEST

With the original parameter values, zero atmospheric emissions input, and depth profiles of carbon and phosphates, the projections of the original Peng '83 model of atmospheric CO₂ declined from 280 ppm in 1860 to 257 ppm in 2300 (Fig. 3). The atmospheric concentrations show relatively large decreases at first and a slower asymptotic decline later. CO₂ concentrations appear to asymptote to the initial partial pressure of CO₂ in the surface layer of ocean.

This nonequilibrium behavior is caused by the discrepancy between the input parameter values and the depth profiles of carbon and phosphate concentrations. As a result, the early behavior of the model is controlled by how far the model is from the equilibrium set by its parameters, rather than by the simulated CO₂ emissions. This shortcoming of the original parameterization influenced only the very early behavior of the model in the verification simulations and scenario projections (Sects. 3.2-3.4).

3.2 REPLICATION OF THE HISTORICAL CO₂ RECORD

The original model was tested with two different sets of historical CO₂ emissions. The first simulation received emissions inputs from both historical burning of fossil fuels and historical land use. The second was run with only the fossil fuel inputs. Historical projections with the original Peng '83 model are shown with the historical measurements in Fig. 4. The model projections in the first case fall below the Siple ice core measurements until the early 1950s and then rise above both the later Siple data and all of the Mauna Loa record. CO₂ projections from the model were compared with the Siple ice core record for the 21 years after 1860 for which Siple measurements were available. The average absolute deviation was 13 ppm. The greatest deviation from the Siple record occurs in 1894, for which the historical projection underestimates the Siple record by 20 ppm.

The historical simulations with only fossil fuel emissions driving the model fit the historical record poorly relative to the combined emissions simulations, but do a better job of reproducing the shape of the CO₂ trajectory. The shape of the simulated atmospheric CO₂ curve is very similar to that of the Siple ice core record, but the projected curve underestimates CO₂ levels by 25-30 ppm throughout. The average absolute deviation is 28 ppm and a maximum deviation of 32 ppm occurs in the year 1927.

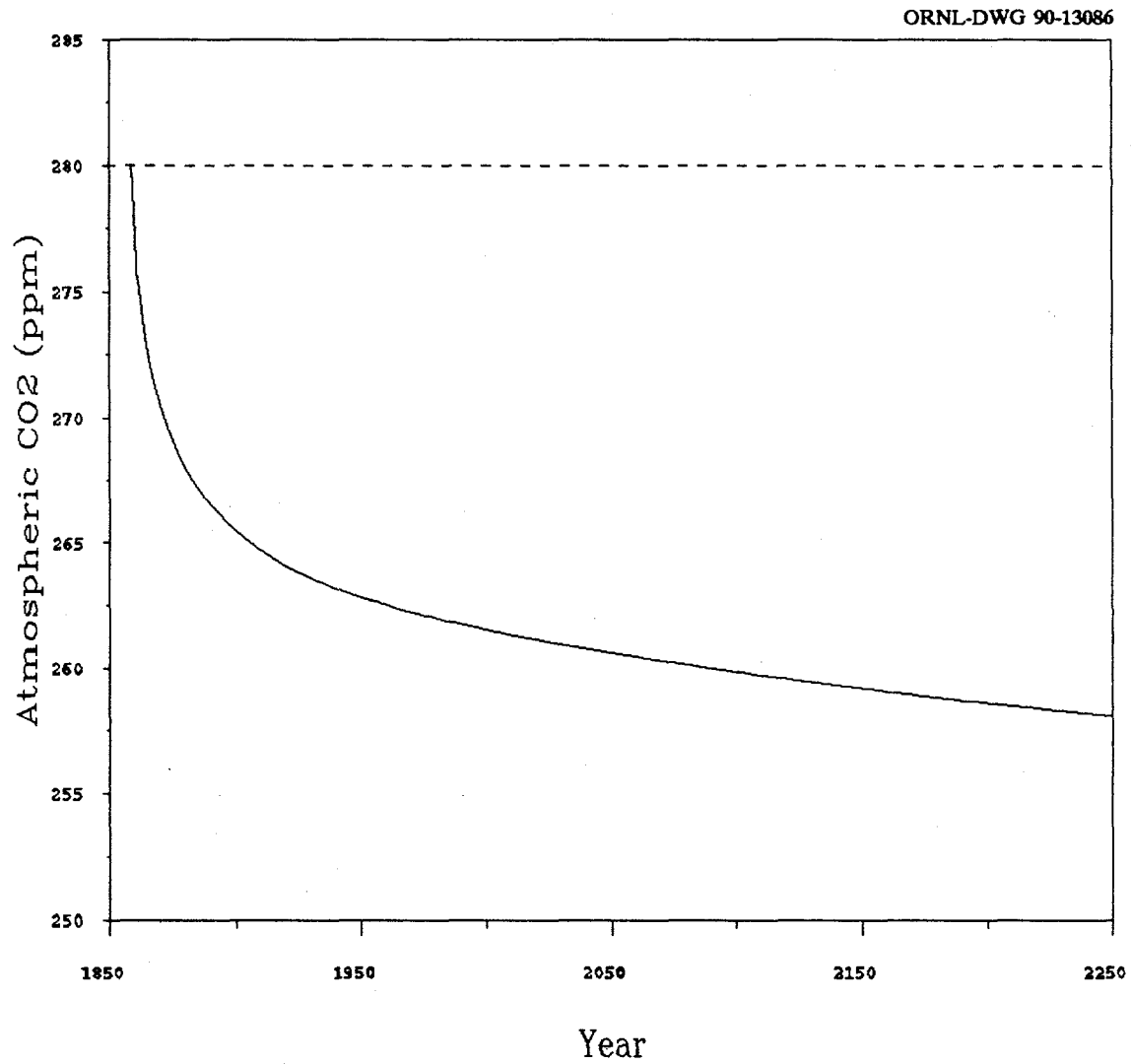


Figure 3. Equilibration test of the original Peng '83 model.

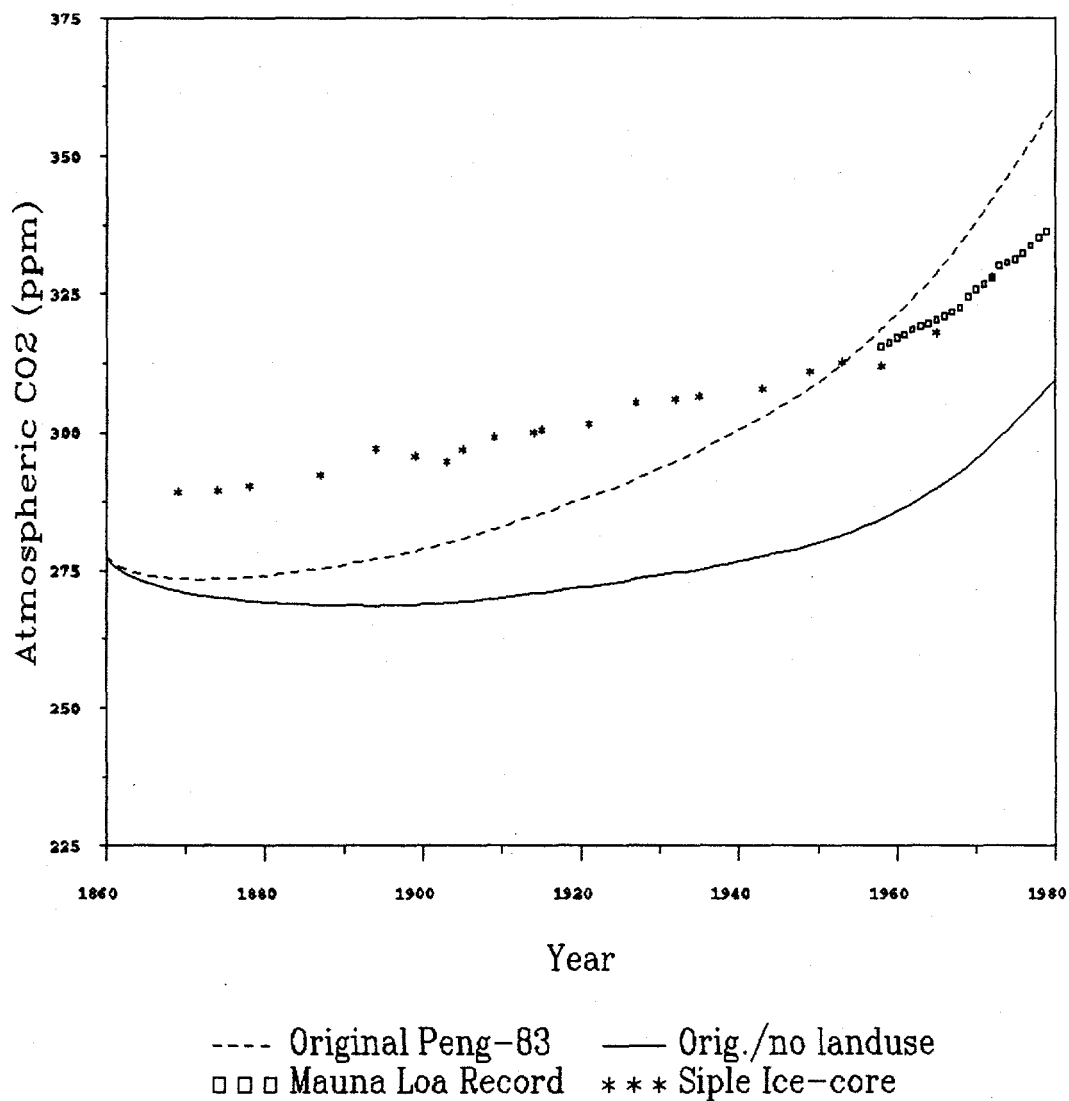


Figure 4. Comparison of historical CO₂ predictions of the original model with the historical CO₂ record.

3.3 REPLICATION OF THE HISTORICAL AIRBORNE FRACTION

Airborne fractions calculated from the historical simulations can be compared with the measured fractions (these so-called "fractions" are expressed as percentages by convention). Measured airborne fractions were calculated over the Mauna Loa and Siple periods, with and without the reconstructed land use emissions. Those calculated without land use were not meaningful ($> 100\%$). Measured airborne fractions of 33% for Mauna Loa and 32% for Siple were calculated from the historical record. The original Peng '83 model estimates airborne fractions of 63% (Mauna Loa period) and 62% (Siple period) when the model is driven by both fossil fuel and land use emissions. With only fossil fuel emissions driving the model, airborne fractions of 65% and 64% are predicted. This result compares favorably with the fraction 61% reported by Baes and Mullholland (1985) for the Peng '83 model. The comparison with measured airborne fractions suggests that all processes that remove carbon from the atmosphere are not included in this model.

3.4 CO₂ FORECASTS

Simulations of nine future emissions scenarios projected by the original Peng '83 model are displayed in Fig. 5. The most apparent feature is the overwhelming importance of the fossil fuel scenario and the relatively minor differences between land use scenarios.

Descriptive statistics that characterize each of the scenario projections are shown in Table 2. As expected, the highest maximum atmospheric CO₂ levels and the earliest doubling and quadrupling times occur for the three high fossil fuel (FF) emissions scenarios, followed by the middle FF scenarios and finally the low FF scenarios. The low FF scenarios do not reach any of the doubling reference concentrations before the year 2300. The three high FF scenarios reach peak atmospheric CO₂ concentrations of ~3500 ppm shortly after the year 2160. The middle FF scenarios for all three LU scenarios do not reach a maximum before the year 2300, and are still increasing. The low FF scenarios peak early at relatively low concentrations. Within each FF scenario, the three land use (LU) scenarios differ slightly, with the middle LU scenarios reaching the highest concentrations, exceeding the high LU scenarios between the years 2100 and 2150. The actual LU emissions of case II exceed those of case I after ca. 2060 (refer to Fig. 9 in section 4.2), so that they are not truly the middle and high LU scenarios throughout the time period.

In general, the higher emissions scenarios generate higher fractions of atmospheric CO₂ that are not taken up by the model ocean. Indices characterizing the projections for the nine emissions scenarios are listed in Table 2.

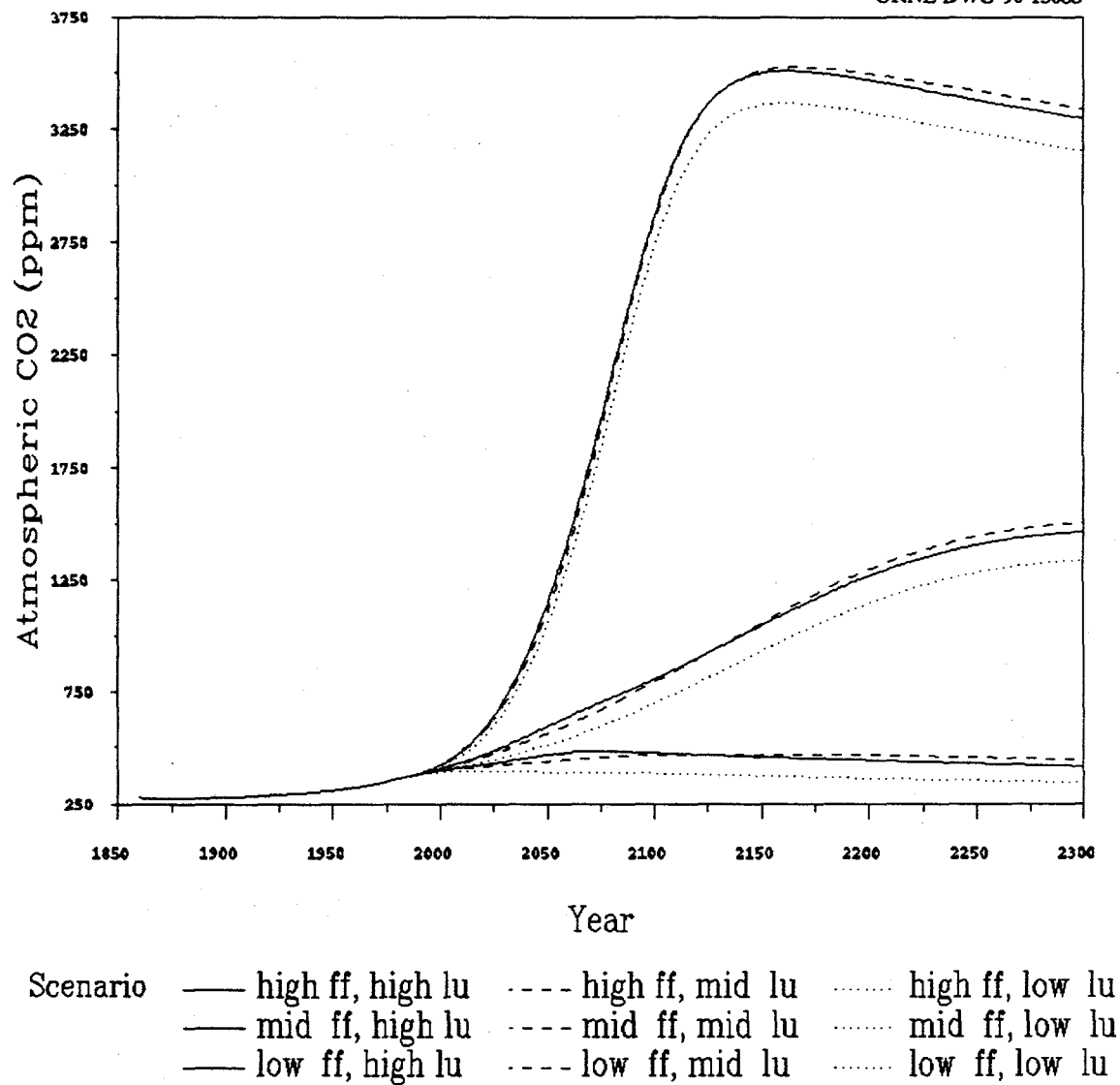


Figure 5. The original model's CO₂ projections for alternative scenarios of future fossil fuel and land use emissions.

Table 2. Descriptive statistics of CO₂ projections made by the original Peng '83 model for nine emissions scenarios.

Statistic	Land use emissions scenario		
	III. (low)	II. (medium)	I. (high)
<i>C. Low fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	391.66	468.73	482.38
Year of Maximum	2010	2135	2076
Reference years		(None reached before 2300)	
Airborne fraction	23.07	33.04	30.31
<i>B. Medium fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	1339.21	1505.00	1464.16
Year of Maximum	2300	2300	2300
Reference years			
600 ppm	2076	2059	2051
680 ppm	2096	2077	2070
1200 ppm	2216	2177	2183
1360 ppm	2300	2218	2229
Airborne fraction	60.70	62.65	62.00
<i>A. High fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	3367.68	3525.99	3509.93
Year of Maximum	2161	2166	2162
Reference years			
600 ppm	2025	2022	2021
680 ppm	2031	2028	2027
1200 ppm	2055	2053	2052
1360 ppm	2061	2058	2057
Airborne fraction	73.42	74.24	74.02

3.5 COMPUTATIONAL REQUIREMENTS

The original Peng '83 model requires around 1.5 min of CPU time for 441 years of simulation. These simulations were run on a VAXStation 3500 operated under VMS V4.7.

PART 2

THE STANDARDIZED PENG '83 MODEL

4. STANDARDIZATION

This work was done as part of a project with the goal of comparing a number of global CO₂ models, one of which the Peng '83 model. The main goal of the standardization process was to allow comparison among CO₂ models by removing any unnecessary differences among them. Standardization attempts to satisfy the following objectives:

1. to use common parameter values in the models;
2. to standardize numerical routines and include them in the model package, where applicable; and
3. to prescribe a common set of initial conditions.

In addition, minimal performance standards were required of the models. Each model was required to pass an equilibration test and to compare reasonably well with the historical atmospheric CO₂ records available from Siple ice core data and from the Mauna Loa records. Meeting these criteria may require modifications or adjustments to the model. In cases in which changes were significant, the original principal investigator or model developer was contacted, and the outcome of the discussions are reported.

4.1 STANDARD PARAMETERIZATION

Table 3 is a list of the nominal parameter values used in the standardized Peng '83 model simulations. Only minor refinements were made to the values used in the original model simulations. The initial condition for the standardized model was set to the 1750 atmospheric concentration of 278 ppm, whereas the original model started in 1860 at 280 ppm.

Table 3. Parameter values of the standardized Peng '83 model

Parameter	Description	Nominal value
AREA	Total ocean surface area	$361 \cdot 10^{12} \text{ m}^2$
CCO2	Polar CO ₂ reaching bottom water	$0.0 \text{ mol} \cdot \text{m}^{-3}$
DD	Depth of deep water origin	1000 m
DKL	Depth of thermocline	700 m
EI	Sea surface CO ₂ exchange rate	$17 \text{ mol} \cdot \text{m}^{-2} \cdot \text{year}^{-1}$
EK	Ocean thermocline diffusivity coefficient	$1.6 \text{ cm}^2 \cdot \text{s}^{-1}$
EKL	Deep sea diffusivity coefficient	$0.5 \text{ cm}^2 \cdot \text{s}^{-1}$
FD	Deep water flux by advection	50 sv
PCO2	Initial atmospheric CO ₂	278 ppm
PPMPM	Conversion from teramoles to ppm	0.00563839218
S	Global average ocean salinity	35 ppt
TW	Global average sea surface temperature	20°C
TALK	Titration ocean alkalinity	$0.00233 \text{ equiv.} \cdot \text{kg}^{-1}$
TCO2	Titration total surface CO ₂ ($\text{mol} \cdot \text{kg}^{-1}$)	0.001969698

4.2 STANDARD EMISSIONS INPUT

Two sources of reconstructed emissions were used to drive the model during the historical period from 1750 to 1980. Reconstructed estimates for fossil fuel emissions reported by Keeling (1973) were used for the historical period from 1750 to 1980. Reconstructed land use emissions were reported Houghton et al. (1983) and Houghton (personal communication) from 1820 to the present. Land use estimates prior to 1820 were obtained by extrapolation to an assumed value of zero in the year 1750. Three future scenarios (high, mid, and low) for fossil fuel emissions were obtained by expanding scenarios defined by Edmonds et al. (1986). Three future scenarios for land use emissions were also based on estimates reported by Houghton et al. (1983). The procedures for defining these scenarios are described in King and Sale (1989). The combinatorial of fossil fuel emissions and land use emissions yields a total of nine scenarios, which were simulated from years 1980 to 2300 (Figs. 6 and 7).

4.3 PROBLEMS AND SOLUTIONS

The main problem addressed in standardizing the Peng '83 model was the calibration of parameters to the desired initial conditions, forcing the model to start at equilibrium. One of the modeling assumptions was that the emission inputs from preindustrial times were low and relatively constant. This assumption allowed the models to start from an

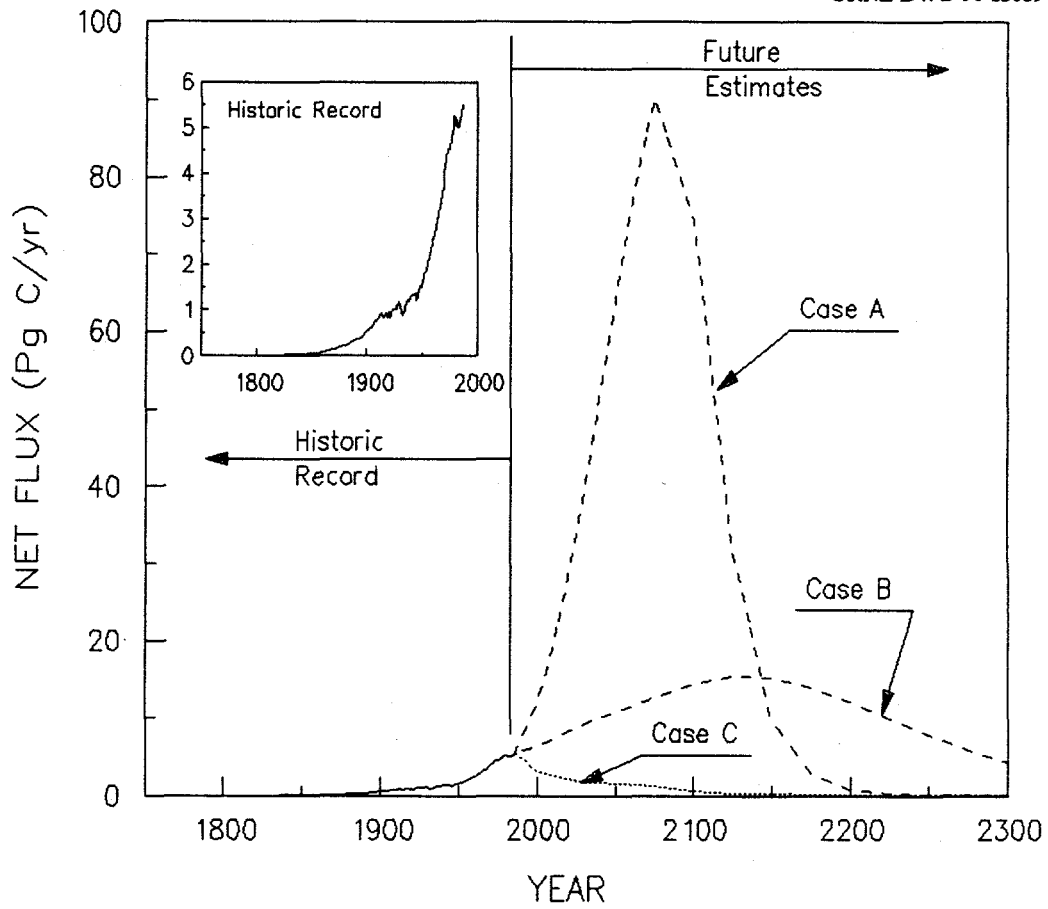


Figure 6. Standardized fossil fuel emissions: reconstructed historical record and three future scenarios.

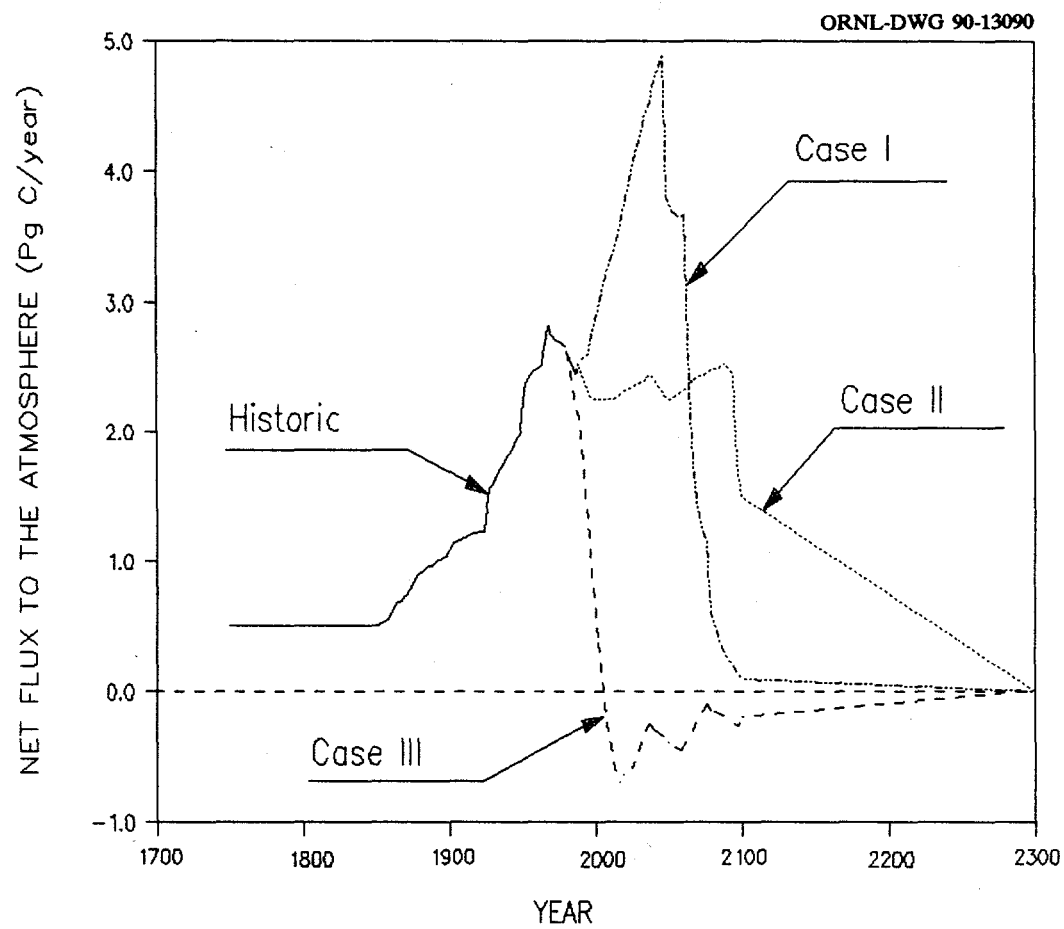


Figure 7. Standardized land use emissions: reconstructed historical record and three future scenarios.

equilibrium baseline condition. The original model did not meet this assumption, which required two changes to the model for the standardized version.

Two phases of equilibration occur in this model: (1) equilibration between atmospheric CO_2 and total ocean CO_2 and (2) equilibration among the 76 ocean layers. Equilibration of the first type is possible in this model only when ocean surface pCO_2 is equated to atmospheric pCO_2 . Preserving the chemical balance in the surface ocean requires selection of a particular value of surface titration total CO_2 in Takahashi's algorithm. In the Peng '83 model, the initial carbon concentration of the mixed-surface layer was used as titration total CO_2 (TALK) in Takahashi's algorithm. The initial mixed layer concentration provided was $1.9697 \mu\text{mol}\cdot\text{kg}^{-1}$. The value required to equilibrate the model with an average ocean temperature of 20°C and a salinity of 35 ppt, respectively, and a total alkalinity of $.00233 \text{ equiv}\cdot\text{L}^{-1}$ is $1.9935 \mu\text{mol}\cdot\text{kg}^{-1}$.

Equilibration among ocean layers in this model requires an equilibrium depth profile for carbon and phosphorus to be determined as a function of the model parameters before projections are made (see subroutine EQUIL in Appendix C). These depth profiles can be determined by solving a linear system of 74 equations that describe the interactions among depth layers at equilibrium. One system of equations pertains to carbon and another to phosphorus, both of which require the concentration in the first and second mixed-surface layers to be known. For carbon, the surface concentration required for ocean-atmosphere equilibration is obtained from Takahashi's algorithm. For phosphorus, the two surface values are set at zero and the concentration of the third layer is set at the original value provided.

5. MODEL VERIFICATION: METHODS

5.1 BASIS FOR VERIFICATION

Several verification criteria have been identified for CO₂ models. Generally, ocean models are expected to reproduce the GEOSECS ocean profiles for natural radiocarbon ¹³C, fossil fuel CO₂, and bomb-produced ¹⁴C (Broecker et al. 1980). Matching these measured profiles indicates that the model ocean dynamics remove each carbon species from the atmosphere and allow it to penetrate the ocean at the same rate as has been observed. This aspect of model verification or calibration was performed by Peng et al. (1983) and led to several of the parameter choices in Tables 1 and 2.

The criterion used here for model verification is the adequate simulation of atmospheric CO₂ over the historical period of the Siple ice core data and the Mauna Loa record. Methods used in comparing model projections with the historical records were described in Sects. 2.3 and 2.4. CO₂ projections were simulated with the standardized model by using each of the nine emissions scenarios shown in Fig. 5-7 (see Sect. 2.5). Several indices summarizing these projections were defined in Sect. 2.5 as well.

5.2 EQUILIBRATION TEST

An important assumption in CO₂ models is that atmospheric CO₂ concentrations were relatively constant during preindustrial times. Without this assumption, it would be necessary to know the amounts of carbon in each depth layer at each starting date in order to specify the initial conditions adequately. Instead, it can be assumed that the carbon allocation among ocean depth layers had reached an equilibrium and, further, that the model dynamics are realistic enough to reproduce the actual equilibrium.

There is an implicit assumption that the simulation starting date is preceded by a constant atmosphere over a significant period of time and by zero emissions. Earlier studies and simulations use 1860 as a typical starting date. The Siple ice core record goes back to earlier dates and suggests that the concentration in the atmosphere was already rising before 1860. Two starting dates are used in the simulations here. Our simulations with the standardized model are run from 1860, for comparison with previous results and the original model, and from 1750 in order to be consistent with this new information and the initialization assumptions.

The equilibration test consists of checking that atmospheric CO₂ remains at the prescribed initial concentration over time when CO₂ emissions are identically zero.

6. MODEL VERIFICATION: RESULTS AND DISCUSSION

6.1 EQUILIBRATION TEST

As part of the standardization process, initial parameter values were calibrated to be consistent with the model's prehistoric equilibrium. The standardized model remained at its initial concentration when emissions were set at zero, and the carbon and phosphorus distributions in the ocean also stayed at their steady-state concentrations.

One feature of these models is that their dynamics allow only a single equilibrium atmospheric (and oceanic) CO₂ concentration corresponding to zero CO₂ emissions and the preindustrial atmospheric concentration. These models are tied to the preindustrial atmosphere, which is the only possible steady-state for the system.

6.2 REPLICATION OF THE HISTORICAL CO₂ RECORD

Historical simulations of atmospheric CO₂ were run for four different cases: (1) starting in 1860 with estimated historical fossil fuel and land use emissions, (2) starting in 1860 with only fossil fuel emissions, (3) starting in 1750 with both fossil fuel and land use emissions, and (4) starting in 1750 with only fossil fuel emissions. Simulations starting in 1860 are shown in Fig. 8, and those starting in 1750 are shown in Fig. 9. The simulations starting in 1860 with 280 ppm are included because these initial conditions are those most-commonly used in the past, before data from the Siple ice-cores were available. In general, the simulations driven by combined fossil fuel and land

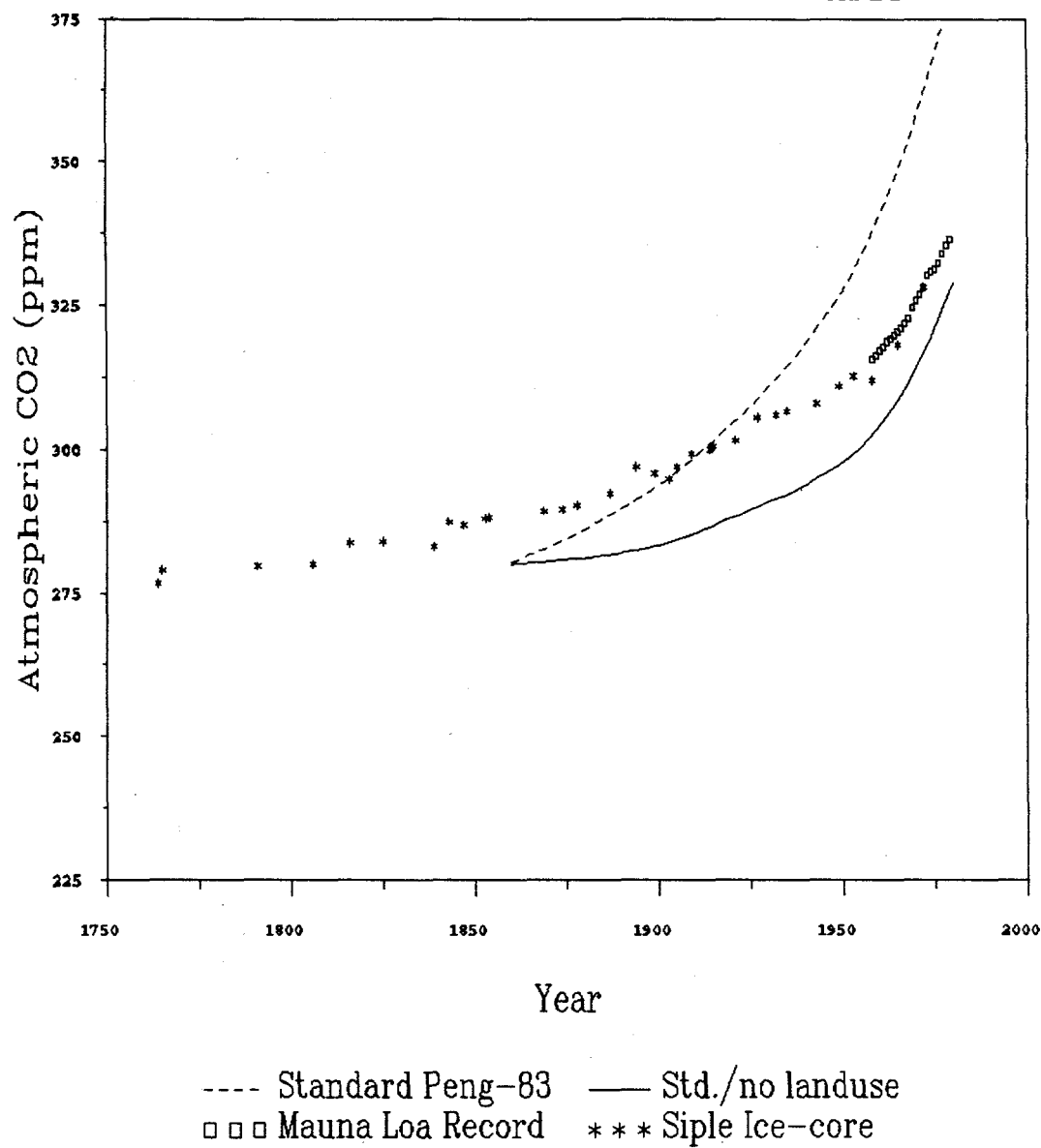


Figure 8. Historical simulation of the standardized Peng '83 model initialized in 1860 with 280 ppm.

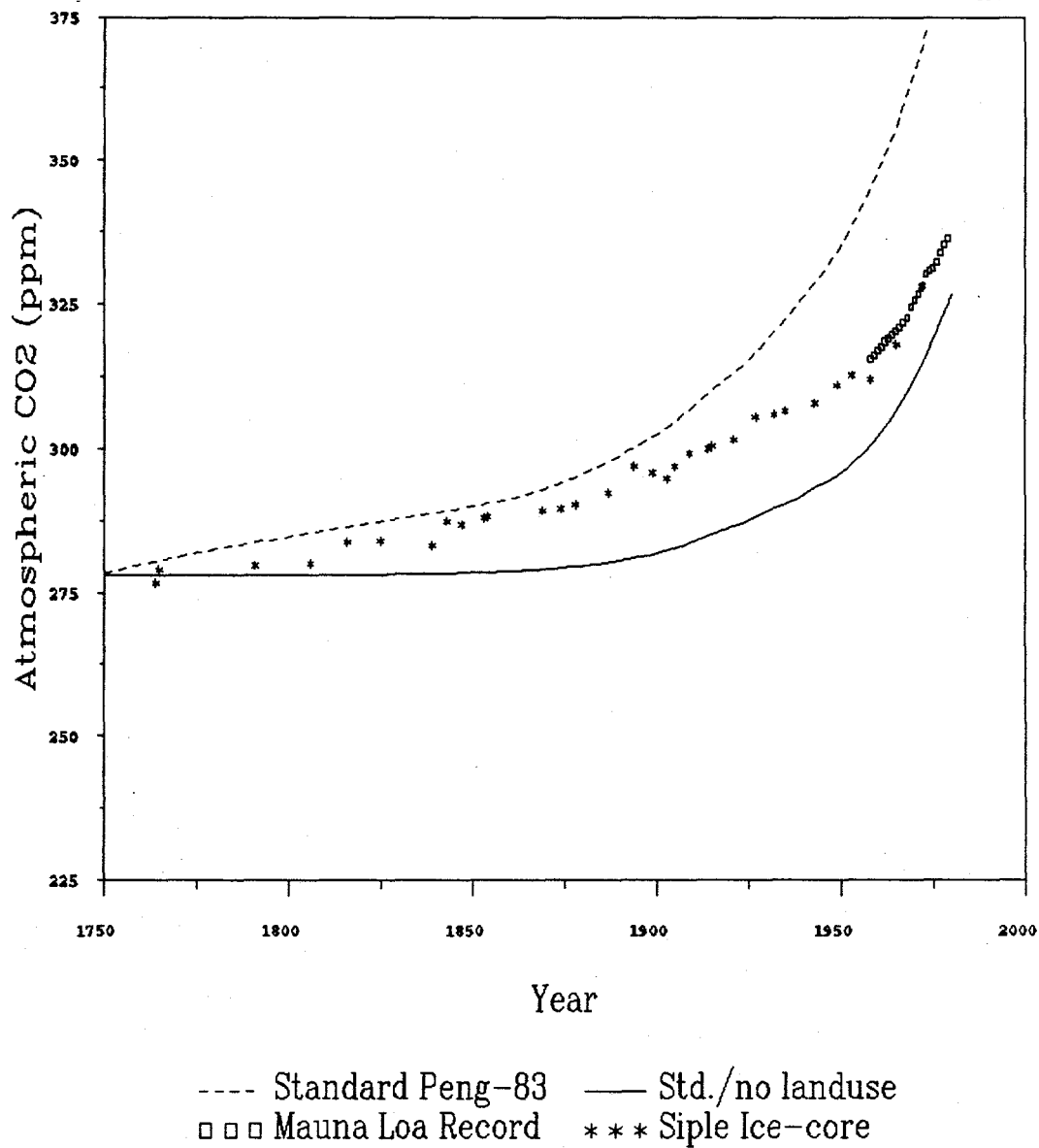


Figure 9. Historical simulation of the standardized Peng '83 model initialized in 1750 with 278 ppm.

use emissions overestimate the observed atmospheric record, and those with only fossil fuel inputs underestimate the observed record. The historical simulation that was initialized at 280 ppm in 1860 and included land use crosses the Siple record in ≈ 1920 and diverges further from the record toward the present. Under the same initial conditions, but with the estimated land use emissions removed, the shape of the trajectory is very similar to the observed record, but underestimates it by about 15 ppm throughout.

The historical simulations started earlier, in 1750, with an initial atmospheric concentration of 278 ppm look qualitatively different from the simulations started later. The observed CO_2 record is bounded below by the simulation without land use and above by the simulation with land use. The combined emission simulation follows the observed data very well until the 20th century, after which both seem to project much faster increases in atmospheric levels than were observed.

The simulated airborne fraction of CO_2 was 42% for the Mauna Loa period (1959-1985) and 59% for the Siple years (1750-1985). These values compare with estimated airborne fractions of around 33%. The tendency for the model to overestimate the retention of CO_2 in the atmosphere should be remembered in evaluating future projections of atmospheric CO_2 . This problem is not unique to this model, but is shared with many other global CO_2 models.

6.3 CO_2 FORECASTS

Forecasts of future atmospheric CO_2 were simulated for nine scenarios of future CO_2 emissions starting in 1750 with $p\text{CO}_2 = 278$ (Fig. 10). The scenarios were discussed in Sect. 2.5 along with the CO_2 forecasts made with the original model. The results here are very similar. The failure to equilibrate immediately in the original model is adjusted for in the historical period and has little apparent impact on future projections. The descriptive statistics in Table 4 summarize the predicted effects of each emissions scenario.

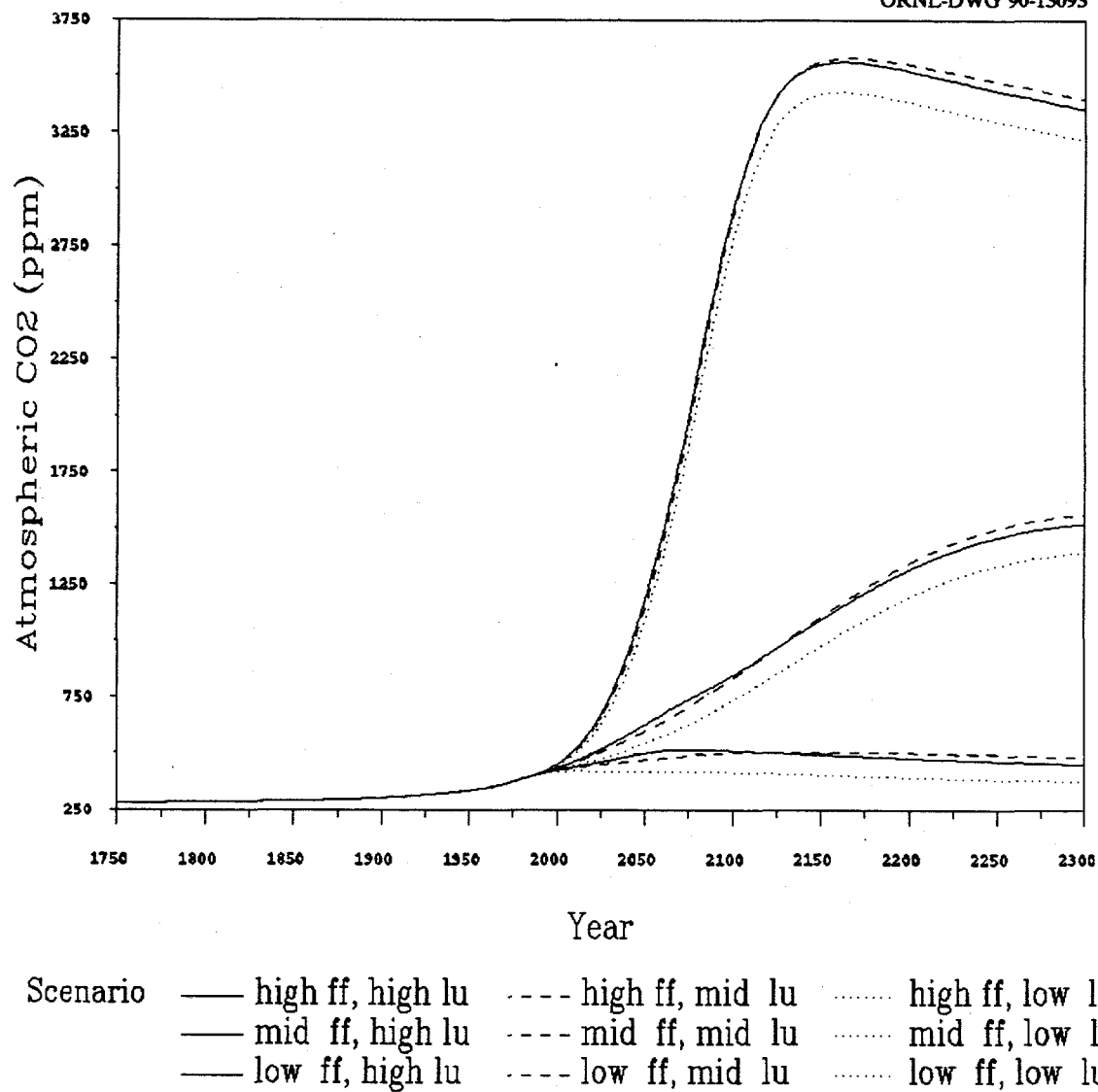


Figure 10. The standardized model's CO₂ projections for alternative scenarios of future fossil fuel and land use emissions.

Table 4. Descriptive statistics of CO₂ projections made by the standardized Peng '83 model for nine emissions scenarios.

Statistic	Land use emissions scenario		
	III. (low)	II. (medium)	I. (high)
<i>C. Low fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	421.61	503.67	516.31
Year of Maximum	2011	2143	2076
Reference years	(None reached before 2300)		
Airborne fractions (%)	32.39	38.96	36.74
<i>B. Medium fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	1392.23	1559.72	1518.61
Year of Maximum	2300	2300	2300
Reference years			
600 ppm	2067	2050	2043
680 ppm	2087	2069	2061
1200 ppm	2202	2168	2172
1360 ppm	2267	2203	2212
Airborne fractions (%)	62.95	64.73	64.12
<i>A. High fossil fuel emissions</i>			
Maximum CO ₂ (ppm)	3429.28	3579.17	3563.00
Year of Maximum	2161	2166	2160
Reference years			
600 ppm	2022	2020	2019
680 ppm	2028	2026	2025
1200 ppm	2054	2051	2050
1360 ppm	2059	2057	2056
Airborne fractions (%)	74.65	75.22	75.00

6.4 COMPUTATIONAL REQUIREMENTS

The standardized Peng '83 model has a calibration routine at the start to ensure equilibrium initial conditions and is therefore expected to take a bit longer than the original model. The standardized version requires a little over 3 minutes of CPU time to run 551 years. The original model required 1.5 min for 441 years.

7. SENSITIVITY ANALYSIS

7.1 INTRODUCTION

Sensitivity analysis serves an important role in model development and understanding. The analysis identifies the relative importance of each parameter on the model predictions of atmospheric CO₂. This information is valuable in deciding which processes included in the model will benefit most from elaboration or improvement. This can prevent spending a large amount of effort in refining aspects of the model that have little influence on the projections or in collecting data for parameters that are unimportant.

In a dynamic model such as the standardized Peng '83 model, it is also interesting to observe changes in parameter importances through time. Usually, parameters that represent initial conditions are very important early in the simulation but soon become unimportant to the later projections.

7.2 METHODS

The parameters listed in Table 3 were included in the sensitivity analysis. A modular software program, Prism, developed at Oak Ridge National Laboratory, was used to conduct the analysis (Gardner and Trabalka 1985; Gardner et al. 1983).

The first module, Prism1, produces a latin-hypercube sample of parameter values having mean values equal to the nominal values in the table (with the exception of CCO₂ = 0.822×10^{-6}) and standard deviations set to 1% of the mean. There was minimal correlation among parameters (max = 0.19). A sample of 250 parameter vectors was drawn.

The second module, Prism2, is the Peng '83 model, which has been modified to read in one vector of parameters at a time, producing atmospheric CO₂ projections for each parameter set. The atmospheric concentrations were saved at 10-year intervals and associated with the parameters that produced them for each of the 250 iterations.

The third module, Prism3, calculates the Pearson correlation between each CO₂ concentration and each parameter. Because the parameters are nearly uncorrelated, the Pearson correlation is close to the relative partial sum of squares (RPSS). The RPSS estimates the additional variance explained by each parameter, given that all other parameters are in the model. For sensitivity analysis, the sum of the RPSS_i should be near 1 for uncorrelated parameters.

A second analysis was run without varying the initial condition, pCO₂. The variability in model projections for this analysis is propagated from variability in the remaining 14 parameters.

7.3 RESULTS AND DISCUSSION

The sensitivity analysis showed the initial $p\text{CO}_2$ to be of overwhelming importance, with a squared partial correlation of nearly 1. This explains why shifting $p\text{CO}_2$ is such an effective method for tuning a CO_2 model to match the historical atmospheric CO_2 record. However, there is little uncertainty in the pre-industrial concentration of (initial) atmospheric CO_2 . This fact underlines the need for using correct initial conditions and looking elsewhere for ways to improve model fit to the historical record.

Relative sensitivities of parameters other than the initial condition were obtained by setting the initial $p\text{CO}_2$ constant and observing the effects of those remaining (see Figs. 11 and 12). In this analysis, global ocean area (AREA) and the exchange rate of CO_2 with the atmosphere (EI) are the most important the first year, 1750. By the year 1760, surface ocean alkalinity (TALK) has become second in importance (23%), while AREA has become first (61%) and EI third (14%). EI soon becomes unimportant, replaced in the rankings by the diffusion coefficient of the upper ocean (EK) which explains 6% of the variation. This new ranking persists, with AREA and TALK the two most important parameters together explaining over 75% of the variation in atmospheric CO_2 , followed by EK, EI, and other parameters of minor importance. The sum of squared correlations ($\times 100\%$) can exceed 100% because of the remaining correlations between parameters and non-linear model behavior. These factors can also cause the sum to be smaller than 100%.

The second analysis revealed the importance of the parameter that estimates the surface area of oceans (AREA). This parameter is used only in the geographic extrapolation from the one-dimensional model CO_2 concentrations to total carbon in the ocean and suggests that this extrapolation can result in large errors. The surface ocean alkalinity is second in importance and may warrant a closer look. A better procedure for determining the global average alkalinity may be required. It is significant that temperature does not appear as important as the alkalinity and exchange rate. The initial importance of EI (29%), and its subsequent decline in importance (4%) probably reflects the influence that this parameter has on the calibration of carbon and phosphorus profiles determined at the outset in the equilibration routines.

The variation in atmospheric CO_2 as a result of a 1% parameter variation increases with time. The variation in CO_2 for the year 1750 is only $.1777 \times 10^{-3}$, whereas the variation has increased to .19% of the mean CO_2 concentration by the year 1980, despite increasing mean concentrations. At the end of the first year, projections vary so little and are dominated by $p\text{CO}_2$ to such an extent that the regression has numerical difficulties. This difficulty is another indication of the overwhelming importance that the initial atmospheric $p\text{CO}_2$ has on the projections.

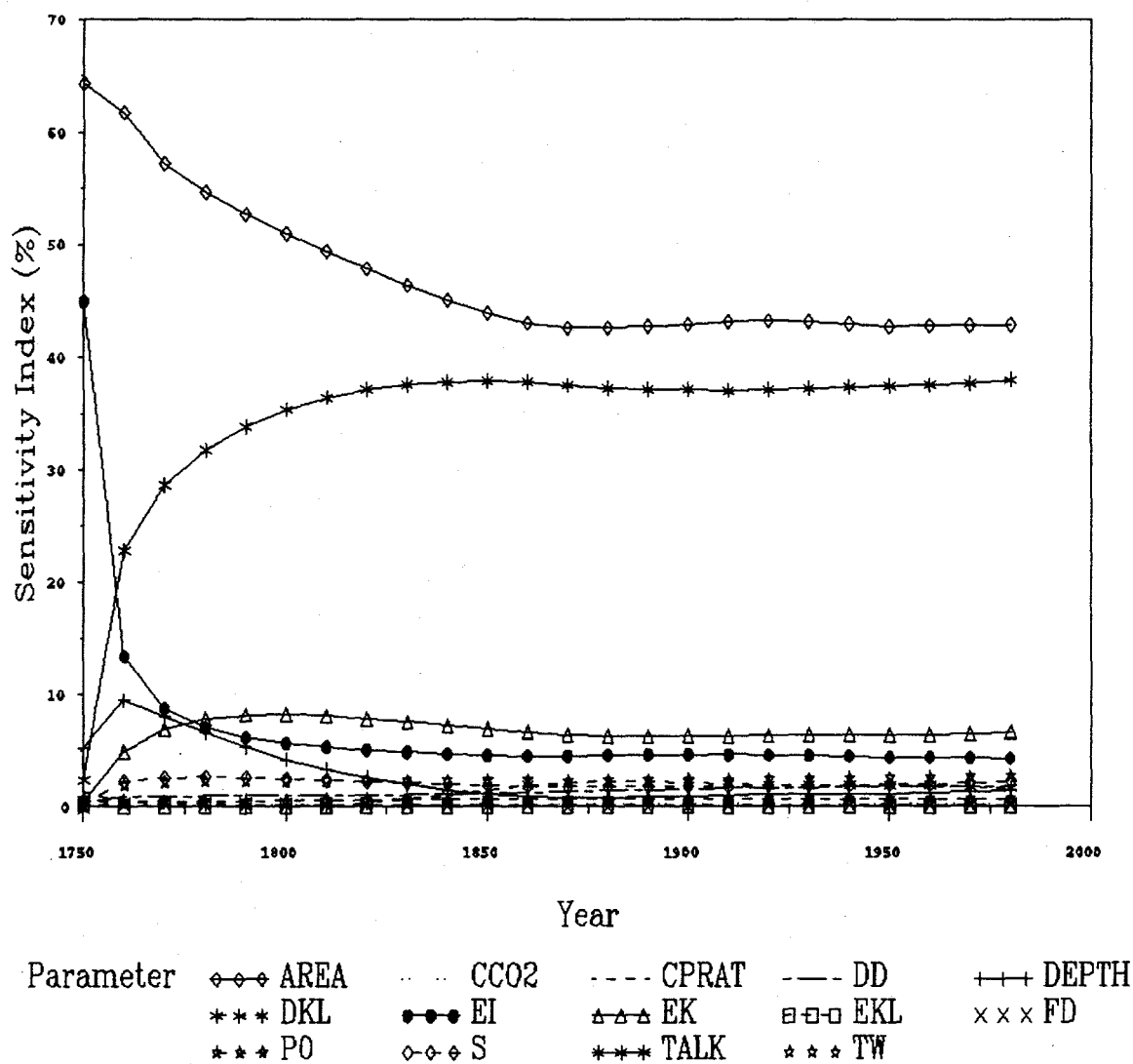


Figure 11. Sensitivity of atmospheric CO₂ projections to Peng' 83 parameters, excluding initial pCO₂ (variable names are defined in Table 1).

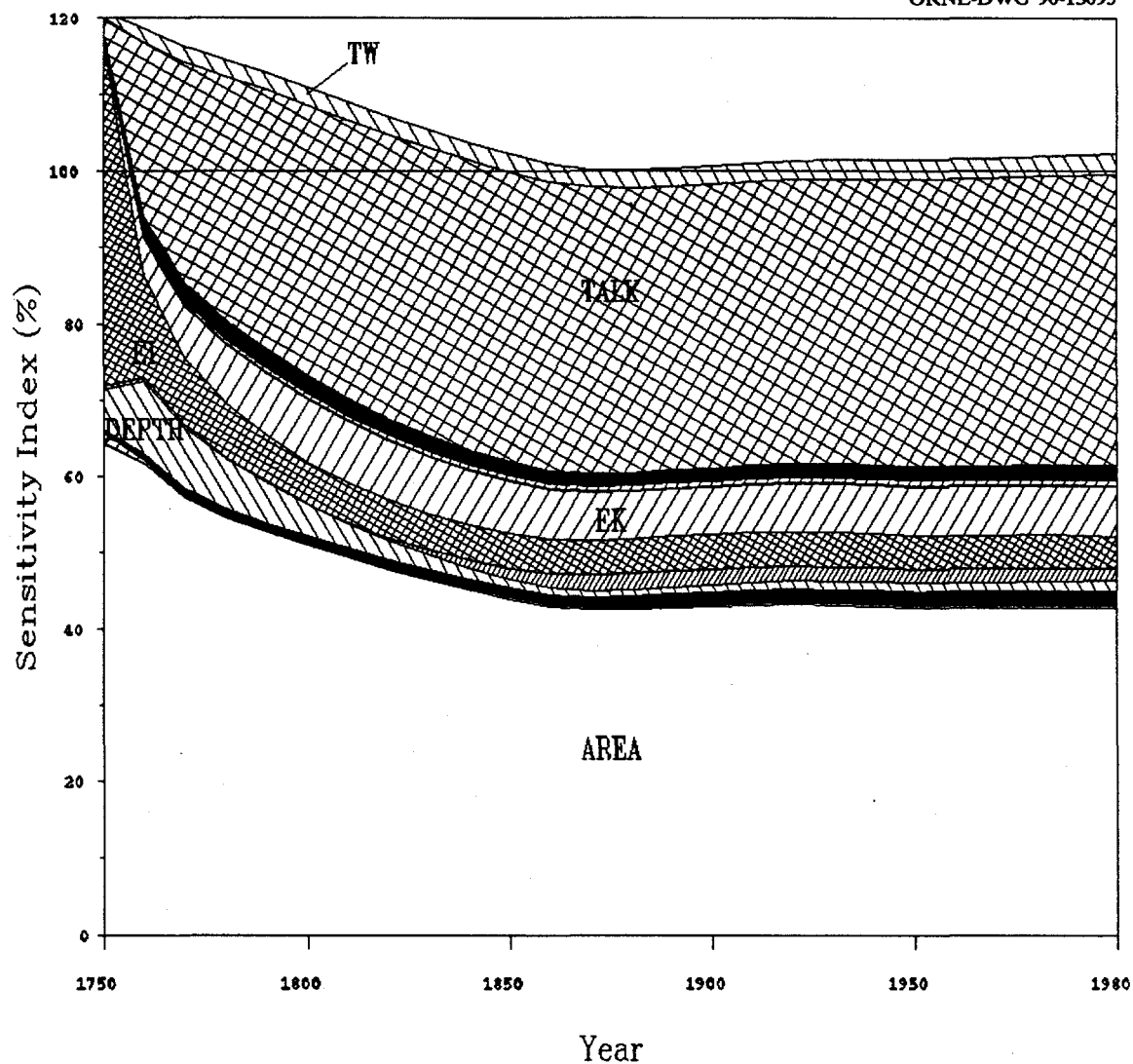


Figure 12. Sensitivity of atmospheric CO₂ projections to model parameters during the historical period 1750-1980 as indicated by shaded areas (see Table 1).

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APPENDIX A

SOURCE CODE LISTING OF THE ORIGINAL MODEL

A.1 MAIN PROGRAM--FFCO2

```
C
C      Name: ffco2.f4, need: rev.f4, dpco2x.f4
C              changes made for ibm
C
C      Purpose: to calculate pco2 in atm and ocean due to ffc
C      input assume constant ffc production rate after 1978
C
C      W.S.Broecker ocean model for co2 uptake (modified
C      Oeschger model) with mixing, upwelling, deep water
C      formation, organic matter production and dissolution
C
C      Note that this version is intended to start in 1860 with
C      co2=280.
C
C      implicit real*8 (a-h,o-z)
C      dimension yr(500),ffc(500),c(76),cc(76),dh(76),a(76)
C      dimension co2x(16),fp(76),bb(76),bp(76),p(76),pp(76)
C      dimension rk(76)
C
C      data t/0.10D0/
C      data tco2w/1.993504D0/,tco2c/2.138670D0/
C      data revf/10.0D0/,iz/0/,tw/20.0D0/,tc/2.0D0/
C      data s/35.0D0/,pco2/280.D0/,talk/0.002330D0/
C
C      key=0 for Oeschger, key=1 for Broecker
C
C      read(5,2) key
C      format(i1)
C1     format(' enter diffu k-top (cm2/s, k<2.)')
C      read(5,10) ek
C2     format(' enter k-low (cm2/s)')
C      read(5,10) ekl
C3     format(' enter depth k-t to k-l (m)')
C      read(5,10) dkl
C      kl=dkl/50.D0
C      kl1=kl-1
C4     format(' enter gas exch e(mole/m2/y)')
C      read(5,10) ei
C7     format(' enter deep water flux(sv)')
C      read(5,10) fd
C8     format(' enter depth deep origin(m), max 3750')
C      read(5,10) dd
C10    format(f15.5)
C      format(' enter polar co2 to bottom water (m/m3)')
C      read(5,10) cco2
C      format(' enter first and last years to simulate')
C
C      read(5,*) ifyr,ilyr
C      year1 = float(ifyr)
C      year2 = float(ilyr)
```

```

c
c read historical and future co2 emmissions record
c including fossil fuel, land use, and cement production,
c convert from e15 grams to units of e12 moles carbon.
c
      open (unit=1,status='old')
      open (unit=2,status='old')
      nyr = 0
20    read (1,*,end=101) iyr,ffin
      read (2,*,end=101) jyr,cluse
      if (iyr .ne. jyr) then
+        write (6,*) 'mismatch in years between',
          ' ffuel & landuse'
        write (6,*) ' at years:',iyr,jyr
        stop
      end if
      if (iyr .Lt. Ifyr .Or. Iyr .Gt. Ilyr) go to 20
      nyr = nyr + 1
      yr(nyr) = float(iyr)
      ffc(nyr)=(ffin+cluse)*1000.D0/12.D0
      go to 20
101   continue
c
c print input parameter values
c
      if (key .Eq. 0) Then
        write(6,29)
      else
        write(6,31)
      end if
29    format('// broecker ocean model')
31    format('// oeschger et al model')
      write(6,17) ek
17    format(' diffu k-t(cm2/s, k<2.) = ',F7.2)
      Write(6,19) ekl
19    format(' diffu k-l(cm2/s, k<2.) = ',F7.2)
      Write(6,21) dkl
21    format(' depth 2-k divide (m) = ',f6.1)
      Write(6,23) ei
23    format(' gas exch e(mole/m2/y) = ',f6.1)
      Write(6,25) fd
25    format(' deep water flux(sv) = ',f6.1)
      Write(6,26) dd
26    format(' depth deep origin(m) = ',f6.1)
      Write (6,122) cco2
122   format(' polar water to deep flux (mole/m3)',g12.4)
      Write (6,123) ifyr,ilyr
123   format(' fossil fuel record entered for ',i4,'-',i4)

      write (6,124) ilyr
124   format(' projections made to year ',i4)
      rkt = ek*3153.6D0/(50.D0*50.D0)*t

```

```

      rkl=ekl*3153.6D0/(50.D0*50.D0)*t
      do 12 i=1,k11
12      rk(i)=rkt
      do 13 i=k1,76
13      rk(i)=rkl
      rw=fd*1.D6*3.1536D7/3.61D14/50.D0*t
      kd=dd/50.D0
      kd1=kd-1
      ia=1.0D0/t
      do 114 i=1,76
          read (5,*) c(i),p(i)
          bp(i)=p(i)
114      bb(i)=c(i)
c
c Top thermocline PO4 released=tor% of total falling
c from mixed layer PO4 releases drop exponentially with depth,
c half oxidation of 400m
c
      tor=8.3D0
      hd=400.D0/50.D0
      tfp=0.0D0
      do 28 i=3,76
          fp(i)=tor*dexp(-0.693147D0/hd*(i-3))
          tfp=tfp+fp(i)
          if(tfp.Gt.100.D0) go to 30
28      continue
      i=76
30      fp(i)=100.D0-(tfp-fp(i))
      ik=i+1
      if(ik.Gt.76) Go to 40
      do 35 k=ik,76
35      fp(k)=0.0D0
40      tffc=0.0D0
      pco2a=pco2
      tco2s=c(1)/1000.D0
c      call dpco2x(iz,tw,s,0.2D-6,1.D-6,talk,tco2s,co2x)
      call dpco2x(iz,tw,s,talk,tco2s,co2x)
      pco2s=co2x(1)*1.D6
c      pco2s=pco2
      write (6,*) '          pco2s=',pco2s
      re=ei/50.D0*t
      tfcs=0.0D0
      write(6,41)
41      format('/' years          sw-pco2          atm-pco2 f-keeling
tffc(e12m)',
*          ' penet(m)          age(y) rev-f')
c
c Project forward in time
c
      do 100 j=1,nyr
          delca=ffc(j)/ia
c          delca=ffc(j)

```

```

delp=delca/5.D4*280.0D0
tffc=tffc+ffc(j)
c
c Mean square root age
c
      tage=0.D0
      do 52 k=1,j
52      tage=tage+(j+1-k)**0.5D0*ffc(k)
      if (tffc .Gt. 0) Age=(tage/tffc)**2.D0
      do 75 l=1,ia
54      pco2a=pco2a+delp
      dpco2=pco2a-pco2s
      rb = rk(2)*p(3)*105.D0/1000.D0
      delcs=dpco2/pco2*re
c      cco2=delcs
42      cc(1)=delcs-rb
      pp(1)=0.0D0
      cc(2)=rk(2)*(c(3)-c(2))
      pp(2)=0.0D0
c fb -- fraction organic diss at each level
      fb=rb/100.D0
      fba=rk(2)*p(3) /100.D0
      do 45 k=3,kd1
          pp(k)=rk(k-1)*(p(k-1)-p(k))+
*          rk(k)*(p(k+1)-p(k))+fba*fp(k)
45      cc(k) = rk(k-1)*(c(k-1)-c(k)) +
*          rk(k)*(c(k+1)-c(k)) + fb*fp(k)
      do 48 k=kd,75
          pp(k)=rk(k-1)*(p(k-1)-p(k))+rk(k)*(p(k+1)-p(k))
*          +rw*(p(k+1)-p(k))+fba*fp(k)
48      cc(k)=rk(k-1)*(c(k-1)-c(k))+rk(k)*(c(k+1)-c(k))
*          +rw*(c(k+1)-c(k))+fb*fp(k)
      pp(76) = rk(75)*(p(75)-p(76)) + rw*(p(kd)-p(76))
*          + fba*fp(76)
      cc(76) = rk(75)*(c(75)-c(76)) + rw*(c(kd)+cco2-c(76))
*          + fb*fp(76)
      do 50 k=1,76
          p(k)=p(k)+pp(k)
50      c(k)=c(k)+cc(k)
      ca=(c(1)+c(2))/2.D0
      c(1)=ca
      c(2)=ca
      tco2s=c(1)/1000.D0
      call rev(iz,tw,s,talk,tco2s,rx)
      revf=rx
      ppc=revf*pco2s*(0.5D0*(cc(1)+cc(2)))/c(1)
      pco2s=pco2s+ppc
      aa=0.0D0
      do 46 k=1,76
          aa=aa+cc(k)
46      pco2a = pco2a-delp + (delca-aa*50.D0*3.6D14/1.D12) /
*          5.D4*280.d0

```

```

75      Continue
c      fk=(tffc-tfcs)/tffc
      ttco2=0.0D0
      sco2=0.0D0
      do 51 i=1,76
          cc(i)=c(i)-bb(i)
          sco2=sco2+cc(i)*50.D0*360.D0
          pp(i)=p(i)-bp(i)
51      ttco2=ttco2+cc(i)*50.D0
      penet=ttco2/cc(1)
      if (tffc .Gt. 0) Fk=(tffc-sco2)/tffc
c      delpf=(pco2a-pco2)/delpz
c
c Print results for each year
c
      write (6,79) yr(j),pco2s,pco2a,fk,tffc,penet,age,revf
79      format (f7.1,F9.2,F10.2,F10.3,1X,g12.4,F10.1,2F8.2)
      Write (7,120) yr(j),pco2a,ffc(j)
120      format (t2,f7.1,2(2X,f10.3))
      If (yr(j) .Eq. 1973.D0) then
132          sco2=sco2*1.D12
          write (6,133) sco2
133          format (/ ' ocean uptake as of 1973 is',e12.4,
*              ' Moles'/)
          end if
100      continue
c
128      borg=50.D0*rk(2)*p(3)*105.D0*ia/1000.D0
      write (6,130) borg
130      format(/ ' organic flux(mole/m2/y)= ',f7.2)
      Stop
      end

```


A.2 SUBROUTINE REV

```
C
C  REV.FOR
C  double precision revelle factor
C  input variables from main program:
C    iz, t(c), s(0/00), talk(eq/kg), tco2(m/kg)
C
C  output variables to main program:
C    r = revelle factor
C
      subroutine rev(iz,t,s,talk,tco2,r)
      implicit real*8 (a-h,o-z)
      dimension cx(16)
      real*4 t,s,talk,tco2,r
      dt=t
      ds=s
      dta=talk
      dtc=tco2
      d=dtc*1.D-6
      tc1=dtc-d
      tc2=dtc+d
      call dpco2x(0,dt,ds,dta,tc1,cx)
      pc1=cx(1)
      call dpco2x(0,dt,ds,dta,tc2,cx)
      pc2=cx(1)
C
C  r=(delta pco2/pco2)/(delta tco2/tco2)
C
      dr=(pc1-pc2)/(pc1+pc2)*(tc1+tc2)/(tc1-tc2)
      r=dr
      return
      end
```

A.3 SUBROUTINE DPCO2X

```

c
c DPCO2X.F4
c double precision
c carbonate chemistry calculations
c
c input variables from main program:
c   z = depth(m)           integer format
c   for solution at p = 1 atm, set z=0
c   t = temperature (c)     real format
c   s = salinity (0/00)     real format
c   talk = titration alkalinity (eq/kg)   real format
c   tco2 = titration total co2 ( m/kg ) real format
c
c output array co2x to main program:
c   co2x(1) = pco2 ( atm)
c   (2) = co3= ( m/kg)
c   (3) = hco3- ( m/kg)
c   (4) = h2co3 ( m/kg)
c   (5) = ah (h+ ion activity)
c   (6) = ph
c   (7) = icp ( (m/kg)**2)
c   (8) = kb (lyman)
c   (9) = k1 (mehrbach et al)
c   (10) = k2 (mehrbach et al)
c   (11) = ksp calcite, p = 1 atm
c   (12) = ksp calcite, p = in situ
c   (13) = co3= (calcite)
c   (14) = ksp aragonite, p = 1 atm
c   (15) = ksp aragonite, p = in situ
c   (16) = co3= (aragonite)
c
c   subroutine dpco2x(z,t,s,talk,tco2,co2x)
c   implicit real*8 (a-h,o-y)
c   integer z
c   real*8 k1,k2,kb,kcalp1,kcalpt,kargp1,kargpt,kw,ksw
c   dimension co2x(16)
c   bas10=dlog(10.00D0)
c   tkt=t+273.15D0
c   k1=dexp(bas10*(13.7201D0-3.1334D-2*tkt-3235.76D0/tkt
c * -1.3D-5*s*tkt+0.1032D0*dsqrt(s)))
c   k2=dexp(bas10*(-5371.9645D0-1.671221D0*tkt-0.22913D0*s
c * -18.3802D0*dlog10(s)+128375.28D0
c * / tkt+2194.3055D0*dlog10(tkt) + 8.0944D-4*s*tkt
c * +5617.11D0*dlog10(s)/tkt-2.136D0*s/tkt))
c   kb = dexp(bas10*(-9.26D0+0.00886D0*s+0.01D0*t))
c
c Pressure effects
c
c   p=1.D0+z*0.1027D0/1.020D0

```

```

      cp=(p-1.D0)/(tkt*83.143D0)
      if(p.Eq.1.)Goto 60
      k1=k1*dexp((24.2D0-0.085D0*t)*cp)
      k2=k2*dexp((16.4D0-0.040D0*t)*cp)
      kb=kb*dexp((27.5D0-0.095D0*t)*cp)
c
60      tb=4.106D-4*s/35.0D0
c
c      alphas = solubility of co2 in seawater (weiss)
c
      tk=tkt/100.D0
      bs=0.023517D0+(-0.023656D0+0.0047036D0*tk)*tk
      alphas = dexp(-60.2409D0+93.4517D0
*          /tk+23.3585D0*dlog(tk)+s*bs)
c
c      Solve for ah by iteration
c
      c1=k1/2.0D0
      c2=1.D0-4.D0*k2/k1
      c4=tb*kb
      ah0=0.75D-8
      do 300 icnt=1,100
      ab=c4/(kb+ah0)
      a=talk-ab
      x=a/tco2
      ah1=c1/x*(1.D0-x+dsqrt(1.D0+c2*x*(-2.D0+x)))
      if(dabs(1.D0-ah0/ah1).Le.0.5D-8) go to 400
300      ah0=ah1
400      continue
c
      co2x(1)=a*(ah1/k1)/(alphs*(1.D0+2.D0*k2/ah1))
      co2x(2)=(a-tco2)/(1.D0-(ah1*ah1)/(k1*k2))
      ca=1.026D-2*s/35.D0
      co2x(3)=tco2/(1.D0+ah1/k1+k2/ah1)
      co2x(4)=tco2/(1.D0+k1/ah1+k1*k2/(ah1*ah1))
      co2x(5)=ah1
      co2x(6)=-dlog10(ah1)
      co2x(7)=ca*co2x(2)
      co2x(8)=kb
      co2x(9)=k1
      co2x(10)=k2
      cv=dexp((36.D0-0.2D0*t)*cp)
      kcalp1=(-34.452D0-39.866D0*s**(1.D0/3.D0) +
*          110.21D0*dlog10(s) -7.5752D-6*tkt*tkt)*1.D-7
      kcalpt=kcalp1*cv
      co3cal=kcalpt/ca
      co2x(11)=kcalp1
      co2x(12)=kcalpt
      co2x(13)=co3cal
      dv=dexp((33.3D0-0.22D0*t)*cp)
      kargp1=1.45*Kcalp1
      kargpt=kargp1*dv

```

```
co3arg=kargpt/ca  
co2x(14)=kargp1  
co2x(15)=kargpt  
co2x(16)=co3arg  
return  
end
```

A.4 INPUT FILE FOR THE ORIGINAL MODEL

```
1           ! 0=Oeschger, 1=broecker model
1.6         ! K-diffusion at top (cm2/s) <= 2
0.5         ! K-diffusion at bottom (cm2/s)
700.        ! Depth = top - bottom (m)
17.         ! Gas exchange e (mode/m2/y)
50.         ! Deep water flux (sv = 1e6 m3/s)
1000.       ! Depth of deep origin (m, < 3750)
0.0         ! Polar co2 to bottom water (m/m3)
1860,1980   ! Initial,final year
```

A.5 PROFILE DATA FOR THE ORIGINAL MODEL

	carbon	phosphate	a
1.969698	0.0		1.001893
1.969698	0.0		1.001893
1.988252	0.176704		1.001707
2.005265	0.338742		1.001539
2.020867	0.487331		1.001387
2.035174	0.623587		1.001250
2.048293	0.748533		1.001126
2.060324	0.863109		1.001014
2.071356	0.968174		1.000912
2.081472	1.064519		1.000819
2.090748	1.152867		1.000735
2.099255	1.233882		1.000659
2.107055	1.308172		1.000590
2.114208	1.376295		1.000526
2.135198	1.576196		1.000343
2.154445	1.759503		1.000179
2.172094	1.927594		1.000030
2.188279	2.081732		0.999896
2.203120	2.223075		0.999775
2.216729	2.352685		0.999665
2.227690	2.457076		0.999578
2.236407	2.540102		0.999509
2.243230	2.605081		0.999455
2.248457	2.654867		0.999414
2.252347	2.691914		0.999384
2.255121	2.718326		0.999363
2.256966	2.735906		0.999348
2.258047	2.746195		0.999340
2.258499	2.750506		0.999336
2.258442	2.749960		0.999337
2.257974	2.745507		0.999341
2.257181	2.737952		0.999347
2.256134	2.727975		0.999355
2.254892	2.716147		0.999364
2.253506	2.702949		0.999375
2.252018	2.688780		0.999387
2.250463	2.673973		0.999399
2.248870	2.658800		0.999411
2.247262	2.643486		0.999424
2.245659	2.628213		0.999436
2.244075	2.613128		0.999449
2.242523	2.598346		0.999461
2.241012	2.583958		0.999473
2.239550	2.570031		0.999484
2.238141	2.556618		0.999495
2.236790	2.543753		0.999506
2.235500	2.531460		0.999516
2.234270	2.519751		0.999526

2.233103	2.508632	0.999535
2.231997	2.498099	0.999544
2.230952	2.488145	0.999552
2.229966	2.478758	0.999560
2.229038	2.469923	0.999567
2.228166	2.461620	0.999574
2.227349	2.453831	0.999580
2.226582	2.446534	0.999586
2.225866	2.439708	0.999592
2.225196	2.433328	0.999597
2.224571	2.427374	0.999602
2.223988	2.421822	0.999607
2.223445	2.416650	0.999611
2.222939	2.411836	0.999615
2.222469	2.407360	0.999619
2.222032	2.403200	0.999623
2.221627	2.399338	0.999626
2.221251	2.395754	0.999629
2.220902	2.392430	0.999632
2.220578	2.389350	0.999634
2.220279	2.386497	0.999637
2.220001	2.383855	0.999639
2.219745	2.381411	0.999641
2.219507	2.379150	0.999643
2.219288	2.377060	0.999645
2.219085	2.375128	0.999646
2.218898	2.373344	0.999648
2.218725	2.371696	0.999649

APPENDIX B
SOURCE CODE LISTING OF THE STANDARDIZED MODEL

B.1 MAIN PROGRAM--PENG.FOR

```

C
C   PENG.FOR
C
C   version modified 12/13/88
C   calculates equilibrium depth profile for c and p
C
C   need: rev.For    - calculates the revelle factor
C               dpco2x.For - Takahashi's ocean chemistry,
C                           calculates pco2s
C               equil.For - calc. equil. depth profiles below
C                           the mixed layer
C               Taka.For  - calc. surface/mixed layer total
C                           carbon, tco2
C
C   Purpose: to calculate pco2 in atm and ocean due to ffc
C           input
C
C   W.S.Broecker ocean model for co2 uptake
C       (modified Oeschiger model) with mixing, upwelling,
C       deep water formation, organic matter production
C       and dissolution
C
C       implicit real*8 (a-h,o-z)
C       dimension yr(600),ffc(600),c(76),cc(76)
C       dimension fp(76),c0(76),p(76),pp(76),rk(76)
C
C   t = model time step, fraction of year
C   secpyr = seconds/year conversion
C   area = total surface area of ocean (m**2) /1.d12
C   ppmppm = ppm/e12-moles conversion (emanuel, 2/14/89)
C   seawgt = weight of 1 cubic meter of sea water (kg)
C
C       data iz/0/,age/0.D0/,fk/0.D0/,t/0.1/
C       data secpyr/3.15576D7/, ppmppm/.00563839218/,
C   *   seawgt/1025.d0/
C       data cmoles/12.011/
C       character*60 rlab, clab*30
C*****
C
C   variable      description
C
C   rlab          title or description of this run (<=60)
C   ek            ocean thermocline diffusivity coefficient
C                 (cm2/s, <2.)
C   ekl          deep sea diffusivity coefficient (cm2/s)
C   dkl          depth of thermocline (m)
C   ei           sea surface co2 exchange rate (moles/m2/yr)
C   fd           flux of deep water (10**6m**3/s=1 sv)
C   dd           depth of deep water origin (m, max 3750)
C   tw           global average sea surface temperature (c)
C   s            global average ocean salinity (pp thousand)

```

```

c pco2          initial pre-industrial atmosphere Co2
c              concentration (ppm)
c talk          alkalinity (eq/kg)
c depth         depth of ocean layers (m)
c area          total ocean surface area (m**2)
c cprat         carbon:phosphorus ratio in organic matter
c p3            conc. of Phosphate below mixed layer p(3)
c
c*****
      read (5,'(a60)') rlab
      read(5,*) ek
      read(5,*) ekl
      read(5,*) dkl
      read(5,*) ei
      read(5,*) fd
      read(5,*) dd
      read(5,*) cco2
      read(5,*) tw
      read(5,*) s
      read(5,*) pco2
      read(5,*) talk
      read(5,*) depth
      read(5,*) area
      read(5,*) cprat
      read(5,*) p3
      read(5,*) ifyr
      read(5,*) ilyr
      year1 = float(ifyr)
      year2 = float(ilyr)
c
c read historical and future co2 emmissions record
c including fossil fuel, land use production,
c convert from e15 grams co2 to units of e12 moles carbon.
c
      open (unit=1,status='old')
      open (unit=2,status='old')
      nyr = 0
20    read (1,*,end=101) iyr,ffin
      read (2,*,end=101) jyr,cluse
      if (iyr .Ne. Jyr) then
*        write (6,*) 'mismatch in years between ffuel',
          ' and landuse'
        write (6,*) ' at years:',iyr,jyr
        stop
      end if
      if (iyr .Lt. Ifyr .Or. Iyr .Gt. Ilyr) go to 20
      nyr = nyr + 1
      yr(nyr) = float(iyr)
      ffc(nyr)=(ffin+cluse)*1000.D0/cmole
go to 20
101  continue
      if (ilyr .Gt. Ifyr+nyr-1) year2=yr(nyr)

```

```

c
c print input parameter values
c
  clab = ' historical emmissions from '
  write (6,'(a30,f7.1)') Clab,year1
  clab = ' co2 projections made to year '
  write (6,'(a30,f7.1)') Clab,year2
  clab = ' diffu k-t(cm2/s, k<2.) = '
  Write(6,'(a30,f7.2)') Clab,ek
  clab = ' diffu k-l(cm2/s, k<2.) = '
  Write(6,'(a30,f7.2)') Clab,ekl
  clab = ' depth 2-k divide (m) = '
  write(6,'(a30,f6.1)') Clab,dkl
  clab = ' gas exch e(mole/m2/y) = '
  write(6,'(a30,f6.1)') Clab,ei
  clab = ' deep water flux(sv) = '
  write(6,'(a30,f6.1)') Clab,fd
  clab = ' depth deep origin(m) = '
  write(6,'(a30,f6.1)') Clab,dd
  clab = ' global avg surface temp= '
  write(6,'(a30,f6.2)') Clab,tw
  clab = ' avg. Ocean salinity = '
  write(6,'(a30,f6.2)') Clab,s
  clab = ' initial atm. Co2 (ppm) = '
  write(6,'(a30,f6.2)') Clab,pco2
  clab = ' alkalinity (eq/kg) = '
  write(6,'(a30,f10.5)') Clab,talk
  clab = ' depth of layers (m) = '
  write(6,'(a30,f6.1)') Clab,depth
  clab = ' ocean surface area (e12-m2)= '
  write(6,'(a30,f6.1)') Clab,area
  clab = ' carbon:phosphorus ratio= '
  write(6,'(a30,f6.0)') Clab,cprat
  clab = ' initial surface p (um/kg)= '
  write(6,'(a30,g12.6)') Clab,p3

c
c assign diffusion rates to each depth layer (1/timestep)
c
  kl=dkl/depth
  kl1=kl-1
  rkt = ek*secpyr*1.D-4*t/(depth*depth)
  Rkl = ekl*secpyr*1.D-4*t/(depth*depth) ! 1/Tth year
  do 12 i=1,kl1
12   rk(i)=rkt
    do 13 i=kl,76
13   rk(i)=rkl
    rw=fd*t*secpyr/(depth*area*1.d6)
    Kd=dd/depth
    kd1=kd-1
    ia=1.0D0/t

c
c top thermocline po4 released=tor% of total falling from

```

```

c mixed layer PO4 releases drop exponentially with depth, half
c oxidation of 400m
c
      tor=8.3D0
      hd=400.D0/depth
      tfp=0.0D0
      do 28 i=3,76
        fp(i)=tor*dexp(-0.693147D0/hd*(i-3))
        tfp=tfp+fp(i)
        if(tfp.Gt.100.D0) go to 30
28      continue
      i=76
30      fp(i)=100.D0-(tfp-fp(i))
      ik=i+1
      do 35 k=ik,76
35      fp(k)=0.0D0
c
c  equilibrate between atmosphere and surface layers of ocean
c
      pco2a=pco2
      pco2s=pco2
c
c  Calculate equilibrium concentrations in depth profiles
c
c... Calculate equilibrium p profile:
c
      p(1) = 0.0d0
      P(2) = 0.0d0
      Fba=rk(2)*p3/100.D0
      call equil(p,rk,fp,rw,fba,0.0,kd)
c
c... Calculate equilibrium c profile based on c(1)=c(2).
c  use takahashi's formulation inverted to get
c  tco2 from pco2 for surface layers, 1 and 2
c
      co2x = pco2s*1.D-6          ! convert from ppm to atm
      Call taka(iz,tw,s,talk,co2x,tco2s)
      c(1) = tco2s*seawgt          ! convert from M/kg to m/m3
      c(2) = c(1)
      clab = ' initial surface c (m/m3)= '
      write(6,'(a30,g12.6)') Clab,c(1)
      dpco2=pco2a-pco2s
      delcs=dpco2*re/280.0d0       ! tied to value of 280
      Rb = rk(2)*p3*cprat*seawgt*1.d-6 ! moles/m3/t
      Fb=rb/100.D0                 ! fraction organic diss
      call equil(C,rk,fp,rw,fb,cco2,kd)
c
c... Save equilibrium profile for c
c
      do 40 k=1,76
40      c0(k) = c(k)
c

```

```

c initialize variables and print headers for time simulation
c
      tffc=0.0D0
      re=ei*t/depth          ! moles/m**3/time step
      write(6,41)
41    format(/t2,'year   emissions      atm.pCo2      sea',
1      ' uptake', '      emission fraction ')
      write(6,42)
42    format(t2, '      (e12-mole)      (ppm)', (e12-mole)',
*      '      ,      sea      air      ')
c
c Project forward in time
c
      do 100 j=1,nyr
        delca=ffc(j)*t      ! Ff flux divided into time steps
        delp=delca*ppmpm ! convert to ppm from E12-moles
        tffc=tffc+ffc(j)
c
c within year simulation
c
      do 75 l=1,ia
54      pco2a=pco2a+delp
        dpco2=pco2a-pco2s
        rb = rk(2)*p3*cprat*seawgt*1.0d-6
        Delcs=dpco2*re/280.0d0 ! mole/m**3/timestep
c
c Calculate fluxes
c
      cc(1)=delcs-rb
      pp(1)=0.0D0
      cc(2)=rk(2)*(c(3)-c(2))
      pp(2)=0.0D0
      fb=rb/100.D0 ! fraction organic diss.
      Fba=rk(2)*p3/100.D0
      do 45 k=3,kd1
        pp(k) = rk(k-1)*(p(k-1)-p(k))
*          + rk(k)*(p(k+1)-p(k))+fba*fp(k)
45      cc(k) = rk(k-1)*(c(k-1)-c(k))
*          + rk(k)*(c(k+1)-c(k))+fb*fp(k)
      do 48 k=kd,75
        pp(k) = rk(k-1)*(p(k-1)-p(k))
*          + rk(k)*(p(k+1)-p(k))
*          + rw*(p(k+1)-p(k))+fba*fp(k)
48      cc(k) = rk(k-1)*(c(k-1)-c(k))
*          + rk(k)*(c(k+1)-c(k))
*          + rw*(c(k+1)-c(k))+fb*fp(k)
      cc(kd) = cc(kd) - rw*cco2 ! balance polar outcrop
      pp(76) = rk(75)*(p(75)-p(76))
*          + rw*(p(kd)-p(76))+fba*fp(76)
      cc(76) = rk(75)*(c(75)-c(76))
*          + rw*(c(kd)+cco2-c(76))+fb*fp(76)
c

```

```

c Add fluxes
c
      do 50 k=1,76
        p(k)=p(k)+pp(k)
50      c(k)=c(k)+cc(k)
        ca=(c(1)+c(2))/2.D0
        c(1)=ca
        c(2)=ca
c
c Recalculate surface and atmospheric pco2
c
      tco2s=c(1)/seawgt          ! moles/kg
      Call rev(iz,tw,s,talk,tco2s,rx)
      revf=rx
      ppc=revf*pco2s*(0.5D0*(cc(1)+cc(2)))/c(1)
      pco2s=pco2s+ppc
c
c recalculate atmospheric co2 by subtracting
c the total amount added to ocean in ppm
c aa*depth*area (e12 moles), converted to ppm
c
      aa=0.0D0
      do 46 k=1,76
46      aa=aa+cc(k)
      pco2a=pco2a - aa*depth*area*ppmpm
75      continue          ! next within-year time step
c
c Calculate yearly statistics, cumulative and by year
c
c   tcatm - cum. atmospheric C      (e12-moles)
c   tsco2 - cum. ocean uptake      (e12-moles)
c   Sco2  - yearly ocean uptake    (e12-moles/yr)
c   ttco2 - cum. ocean uptake      (e12-moles/m2 ocean surface)
c   Tffc  - cum. total emissions   (e12-moles)
c
      Tcatm=(pco2a-pco2)/ppmpm
      old = ttco2
      ttco2=0.0D0
      do 51 i=1,76
        cc(i)=c(i)-c0(i)      ! current-initial C profile
51      ttco2=ttco2+cc(i)
        ttco2=ttco2*depth      ! M/m**2 ocean surface area
        tsco2=ttco2*area       ! e12-Moles c
        sco2 =tsco2-old*area
c
c Calculate seaborne fraction and airborne fraction
c
c   sf = cumulative ocean uptake/cumulative emissions
c   af = cumulative atmos uptake/cumulative emissions
c
      sf = (tsco2/tffc)*100.D0
      af = (tcatm/tffc)*100.D0

```

```
c
c Print results for each year
c
      write (6,79) yr(j),ffc(j),pco2a,sco2,sf,af
79    format (t2,f5.0,3(1x,G12.6),2(2x,f8.2))
c
100   Continue      ! next year
      Stop
      end
```


B.2 SUBROUTINE TAKA

```
c
c  TAKA.FOR - calculates titration total co2 from known
c              pco2s=pco2a.
c
c  double precision
c  carbonate chemistry calculations
c
c  input variables from main program:
c    z = depth(m)                      integer format
c    for solution at p = 1 atm, set z=0
c    t = temperature (c)                real format
c    s = salinity (0/00)                real format
c    talk = titration alkalinity ( eq/kg) real format
c    co2x = pco2 of atmosphere and surface at eq. (Atm)
c
c  output to main program:
c    tco2 = total titration co2 (m/kg)
c
c      subroutine taka (z,t,s,talk,co2x,tco2)
c      implicit real*8 (a-h,o-y)
c      integer z
c      real*8 k1,k2,kb,kcalp1,kcalpt,kargp1,kargpt,kw,ksw
c      bas10=dlog(10.00D0)
c      tkt=t+273.15D0
c      k1=dexp(bas10*(13.7201D0-3.1334D-2*tkt-3235.76D0/tkt
c      * -1.3D-5*s*tkt+0.1032D0*dsqrt(s)))
c      k2=dexp(bas10*(-5371.9645D0-1.671221D0*tkt-0.22913D0*s
c      * -18.3802D0*dlog10(s) +128375.28D0/tkt
c      * +2194.3055D0*dlog10(tkt)+8.0944D-4*s*tkt
c      * +5617.11D0*dlog10(s)/tkt-2.136D0*s/tkt))
c      kb=dexp(bas10*(-9.26D0+0.00886D0*s+0.01D0*t))
c
c  Pressure effects
c
c      p=1.D0+z*0.1027D0/1.020D0
c      cp=(p-1.D0)/(tkt*83.143D0)
c      if(p.Eq.1.)Goto 60
c      k1=k1*dexp((24.2D0-0.085D0*t)*cp)
c      k2=k2*dexp((16.4D0-0.040D0*t)*cp)
c      kb=kb*dexp((27.5D0-0.095D0*t)*cp)
60      tb=4.106D-4*s/35.0D0
c
c  Alphs = solubility of co2 in seawater (weiss)
c
c      tk=tkt/100.D0
c      bs=0.023517D0+(-0.023656D0+0.0047036D0*tk)*tk
c      alphs=dexp(-60.2409D0+93.4517D0
c      * /tk+23.3585D0*dlog(tk)+s*bs)
c      c1=k1/2.0D0
c      c2=1.D0-4.D0*k2/k1
c      c4=tb*kb
```

```

c
c Find [h+] from talk,co2x cubic equation
c convert [h+] = ah = ah*10**6
c
      p = 1.D6*(kb-(c4+alphs*k1*co2x)/talk)
      q = 1.D12*(-alphs*k1*co2x*(2.d0*k2+kb)/talk)
      r = 1.D18*(-2.d0*k2*kb*alphs*k1*co2x/talk)
      a = q-p*p/3.d0
      b = (2.d0*p*p*p-9.d0*p*q+27.d0*r)/27.d0
      chk = b*b/4.d0 + a*a*a/27.d0
c
c chk < 0, should have 3 real roots
c let x = xm cos(theta)
c
      xm = 2.d0*dsqrt(-a/3.d0)
      theta = acos(3.d0*b/(a*xm))/3.d0
      root1 = xm*cos(theta)
      ah = 1.d-6*(root1-p/3.d0)
c
c Solve for tco2 - surface layer carbon concentration
c
      b = ah/c1 + 1.d0
      x = 2.d0*(b-c2)/(b*b-c2)
      tco2 = (talk-c4/(kb+ah))/x
      return
      end

```

B.3 SUBROUTINE EQUIL

```
      Subroutine equil(x,rk,fp,rw,fb,cco2,kd)
C
C  Equil calculates the equilibrium depth profile for x,
C  where x can be carbon or phosphate, based on the other
C  model parameter values and [X] in the surface layer.
C
      Implicit real*8 (a-h,o-z)
      real*8 x(76),rk(76),fp(76)
      real*8 a(76,5)
      real*8 kd2,11,12
C
C... Calculate first two rows of tridiagonal coefficient
C... matrices for C and p as well as the right hand side of
C... the eqn  $ac = b$ .
C... Matrix a: 1st column stores lower diagonal of a,
C...             2nd column stores diagonal,
C...             3rd column stores upper diagonal.
C...             4th column stores r.h.s. (photosynthesis)
C...             A also has entry 76,kd=rw, which is not stored.
      do 20 i=1,76
        do 20 j=1,5
          a(i,j) = 0.0d0
20    continue
C
C Surface two layers (up to 75 m)
C
C... Combine rows (compartments) 1 and 2, since they are
C... equal. The new row 2 for carbon is [0 -rk2 rk2 0 0
C... |rb-delcs], but ends up singular, so just assign original
C... c(2)=c(1).
C... For phosphorus, p(1)=p(2)=zero, assign p(3).
C
      A(2,2) = 1.0d0
      A(2,4) = x(2)
C
C Thermocline layers (to kd)
C
      do 45 k=3,kd-1
        a(k,1) = rk(k-1)
        a(k,2) = -rk(k-1)-rk(k)
        a(k,3) = rk(k)
        a(k,4) = -fb*fp(k)
45    continue
C
C Deep layers of ocean
C
      do 48 k=kd,75
        a(k,1) = rk(k-1)
        a(k,2) = -rk(k-1)-rk(k)-rw
        a(k,3) = rk(k)+rw
```

```

      a(k,4) = -fb*fp(k)
48      continue
      a(kd,4) = a(kd,4) + cco2*rw
c
c   Deepest layer
c
      a(76,1) = rk(75)
      a(76,2) = -rk(75)-rw
      a(76,3) = 0.d0
      a(76,4) = -fb*fp(76)-cco2*rw
c
c... Apply givens rotations to obtain an lower-diagonal coef.
c... matrix zero-out upper off-diagonal of almost tri-diagonal
c... matrix.
c...
c... Shift matrix to left, putting new leftmost diagonal in
c... column 1, subdiagonal in column 2, diagonal in column 3,
c... r.h.s. in column 4, and column cd coefficients in col. 5.
c...
c... k+1 row (except 76th) is already shifted,
c... while kth is not.
c
      Do 50 kk=1,74
      k=76-kk
      l1 = a(k,1)
      d1 = a(k,2)
      u1 = a(k,3)
      if (kk .eq. 1) then ! original positions in A
      l2 = a(k+1,1)
      d2 = a(k+1,2)
      kd2 = rw
      else ! shifted positions in A
      l2 = a(k+1,2)
      d2 = a(k+1,3)
      kd2 = a(k+1,5)
      end if
      call givens(d2,u1,cosa,sina)
c
c
c   | 1 0 0 0 |   | x x 0 0 |   =   | x x 0 0 |
c   | 0 1 0 0 |   | x x x 0 |   =   | x x x 0 |
c   | 0 0 c -s |   | 0 l1 d1 u1 |   =   | 0 cl1 cd1-sl2 0 |
c   | 0 0 s c |   | 0 0 l2 d2 |   =   | 0 sl1 sd1+cl2 su1+cd2 |
c
      a(k,2) = cosa*l1
      A(k,3) = cosa*d1 - sina*l2
      A(k+1,1) = sina*l1
      A(k+1,2) = sina*d1 + cosa*l2
      A(k+1,3) = sina*u1 + cosa*d2
c
c... apply transformation matrix J(k,k+1,theta) to the
c... right-hand side.
c

```

```

        v = A(k,4)
        w = a(k+1,4)
        a(k,4) = cosa*v - sina*w
        a(k+1,4) = sina*v + cosa*w
c
c Deal with intersection between new kdth col and diagonal
c
        if (k .le. kd) then
            A(k,5) = 0.0d0
            go to 50
        end if
        A(k,5) = -sina*kd2
        A(k+1,5) = cosa*kd2
        if (k .eq. kd+2) then
            savekd1 = A(k,5)
        else if (k .eq. kd+1) then
            A(k,2) = a(k,2) + a(k,5)
            a(k+1,1) = a(k+1,1) + cosa*savekd1
        end if
50      continue
c
c... Solve for equilibrium by forward substitution
c... x(i) = (b(i) - (lower diag)x(i-1) - (next lower
c... diag)x(i-2) - (column kd)x(kd)) / diagonal
c
        a(3,1) = 0.0d0
        Do 52 k=3,76
            x(k)=a(k,4)-a(k,2)*x(k-1)-a(k,1)*x(k-2)
            if (k .gt. kd+2) x(k) = x(k) - A(k,5)*x(kd)
            if (a(k,3) .ne. 0.d0) then
                x(k) = x(k)/A(k,3)
            else
                write (6,*) ' system is rank ',76-k
                go to 60
            end if
52      continue
60      continue
        return
        end

```

B.4 SUBROUTINE GIVENS

```
      subroutine givens(v,w,cosa,sina)
      implicit real*8 (a-h,o-z)
c
c  get rid of w = cosa*w - sina*v
c
      if (w .eq. 0.d0) then
        sina = 0.0d0
        cosa = 1.0d0
        return
      end if
      if (dabs(w) .ge. dabs(v)) then
        t = v/w
        sina = 1.d0/dsqrt(1.d0+t*t)
        cosa = sina*t
      else
        t = w/v
        cosa = 1.d0/dsqrt(1.d0+t*t)
        sina = cosa*t
      end if
      Return
      end
```

B.5 SUBROUTINE REV

```
C
C REV.FOR
C double precision revelle factor
C input variables from main program:
C   iz, t(c), s(0/00), talk(eq/kg), tco2(m/kg)
C
C output variables to main program:
C   r = revelle factor
C
      subroutine rev(iz,t,s,talk,tco2,r)
      implicit real*8 (a-h,o-z)
      dimension cx(16)
      real*4 t,s,talk,tco2,r
      dt=t
      ds=s
      dta=talk
      dtc=tco2
      d=dtc*1.D-6
      tc1=dtc-d
      tc2=dtc+d
      call dpco2x(0,dt,ds,dta,tc1,cx)
      pc1=cx(1)
      call dpco2x(0,dt,ds,dta,tc2,cx)
      pc2=cx(1)
C
C   r=(delta pco2/pco2)/(delta tco2/tco2)
C
      dr=(pc1-pc2)/(pc1+pc2)*(tc1+tc2)/(tc1-tc2)
      r=dr
      return
      end
```

B.6 SUBROUTINE DPCO2X

```

C
C DPCO2X.FOR
C modified to yield more precision in h+ iteration
C and remove some unused element calculations.
C carbonate chemistry calculations
C
C input variables from main program:
C   z = depth(m) integer format
C   for solution at p = 1 atm, set z=0
C   t = temperature (c) real format
C   s = salinity (0/00) real format
C   talk = titration alkalinity (eq/kg) real format
C   tco2 = titration total co2 ( m/kg ) real format
C
C output scalar co2x to main program:
C   co2x = pco2 ( atm)
C
      subroutine dpcO2x(z,t,s,talk,tco2,co2x)
      implicit real*8 (a-h,o-y)
      integer z
      real*8 k1,k2,kb,kcalp1,kcalpt,kargp1,kargpt,kw,ksw
      data tiny/1.d-15/
      Bas10=dlog(10.00D0)
      tkt=t+273.15D0
      k1=dexp(bas10*(13.7201D0-3.1334D-2*tkt-3235.76D0/tkt
+ -1.3D-5*s*tkt+0.1032D0*dsqrt(s)))
      k2 = dexp(bas10*(-5371.9645D0
+ - 1.671221D0*tkt-0.22913D0*s -18.3802D0*dlog10(s)
+ + 128375.28D0/tkt+2194.3055D0*dlog10(tkt)
+ + 8.0944D-4*s*tkt + 5617.11D0 * dlog10(s) /
+ tkt-2.136D0*s/tkt))
      kb = dexp(bas10*(-9.26D0+0.00886D0*s+0.01D0*t))
C
C Pressure effects
C
      p=1.D0+z*0.1027D0/1.020D0
      cp=(p-1.D0)/(tkt*83.143D0)
      if(p.Eq.1.)Goto 60
      k1=k1*dexp((24.2D0-0.085D0*t)*cp)
      k2=k2*dexp((16.4D0-0.040D0*t)*cp)
      kb=kb*dexp((27.5D0-0.095D0*t)*cp)
C
60      tb=4.106D-4*s/35.0D0
C
C Alphas = solubility of co2 in seawater (weiss)
C
      tk=tkt/100.D0
      bs=0.023517D0+(-0.023656D0+0.0047036D0*tk)*tk
      alphas=dexp(-60.2409D0+93.4517D0
+ /tk+23.3585D0*dlog(tk)+s*bs)
C

```



```

c  solve for ah by iteration
c
      c1=k1/2.0D0
      c2=1.D0-4.D0*k2/k1
      c4=tb*kb
      ah0=0.75D-8
      do 300 icnt=1,1000
      ab=c4/(kb+ah0)
      a=talk-ab
      x=a/tco2
      ah1=c1/x*(1.D0-x+dsqrt(1.D0+c2*x*(-2.D0+x)))
      if(dabs(1.D0-ah0/ah1).Le.tiny) Go to 400
300   ah0=ah1
400   continue
      co2x=a*(ah1/k1)/(alphs*(1.D0+2.D0*k2/ah1))
      return
      end

```

B.7 INPUT FILE FOR THE STANDARDIZED MODEL

Run of emissions scenarios	!	RLAB
1.6	! K-diffusion at top (cm2/s)	EK
0.5	! K-diffusion at bottom (cm2/s)	EKL
700.	! Depth = top - bottom (m)	DKL
17.	! Gas exchange E (mole/m2/y)	EI
50.	! Deep water flux (sv = 1E6 m3/s)	FD
1000.	! Depth of deep origin (m, < 3750)	DD
0.0	! Polar CO2 to bottom water (m/m3)	CCO2
20.0	! Global avg. sea surface temp (C)	TW
35.0	! Global avg. ocean salinity (ppm)	S
280.0	! Initial atmospheric CO2 (10**-6atm)	PCO2
0.00233	! Alkalinity (eq/kg)	TALK
50.0	! Depth of ocean layers (m)	DEPTH
361.0	! Ocean surface area E12-m2	AREA
105.0	! C:P ratio in organic matter	CPRAT
0.176705	! Third layer initial phosphate P(3)	P0
1750	! Initial year of simulation	YEAR1
2300	! Final year of simulation	YEAR2

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